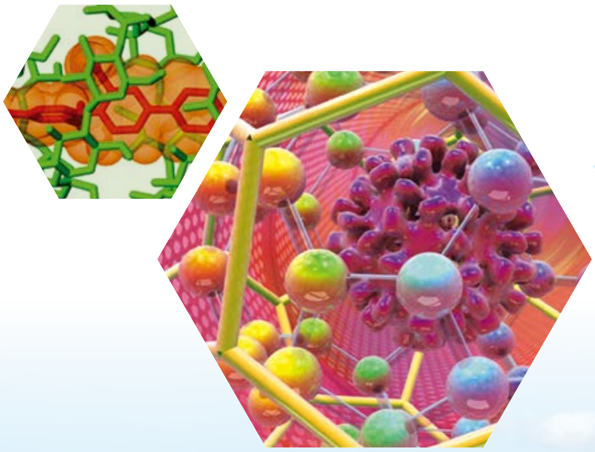
香港科技大學
THE HONG KONG UNIVERSITY OF
SCIENCE AND TECHNOLOGY

HKUST JOCKEY CLUB
INSTITUTE FOR ADVANCED STUDY
香港科技大學賽馬會高等研究院

The 11th International Conference on

Optical Probes of Conjugated Polymers and Organic Nanostructures

14-19 June 2015, HKUST, Hong Kong



HKUST Jockey Club Institute for Advanced Study

The 11th International Conference on Optical Probes of Conjugated Polymers and Organic Nanostructures (OP2015)

14 - 19 June 2015

The Hong Kong University of Science and Technology

Contents

Abstracts

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Conference Schedule

14 June 2015 (Sun) – Pre-conference Tutorial (Seminar on Current Trends and Status of Organic Light Emitting Diode and Organic/ Hybrid Solar Cell)

Time	Event	Venue
08:30-17:00	Registration	Lobby, G/F
09:00-10:30	Talk: "Optical, Electrical and Magnetic Properties of Organic/Inorganic Hybrid Perovskites" Valy Vardeny (The University of Utah)	IAS Lecture Theater, G/F
10:30-11:00	Coffee break	Lobby, G/F
11:00-12:30	Talk: "Plasmonic Organic Solar Cells and LEDs" Wallace C H Choy (The University of Hong Kong)	IAS Lecture Theater, G/F
12:30-14:00	Lunch (Self-arranged)	
14:00-15:30	Talk: "The Physics and Chemistry of Thermally Activated Delayed Fluorescence" Andy Monkman (University of Durham)	IAS Lecture Theater, G/F
15:30-16:00	Coffee break	Lobby, G/F
16:00-17:30	Talk: "OLED Applications: Opportunities and Challenges" Furong Zhu (Hong Kong Baptist University)	IAS Lecture Theater, G/F

15 June 2015 (Mon) - Day 1

Time	Event	Venue
08:30-17:00	Conference Registration	Lobby, G/F
08:50-09:00	Conference Opening	IAS Lecture Theater, G/F
Organic Metamaterial and Lasers **Session Chair:** ***Kam Sing Wong (The Hong Kong University of Science and Technology)***		
09:00-09:45	Plenary Talk#01: "Molecular Metamaterials: Using Polymer Conformation to Define Photonic Nanostructures" Donal Bradley (Imperial College London)	IAS Lecture Theater, G/F
09:45-10:15	Invited Talk#02: "Organic & Hybrid Photonic Crystals: From Lasers to Sensors" Davide Comoretta (Universita di Genova)	
10:15-10:45	Invited Talk#03: "Optical Gain Property Investigation of Novel Green-yellow Emission Polymer F8F5BT and Its Blends with PFO" Ruidong Xia (Nanjing University of Posts and Telecommunications)	
10:45-11:15	Coffee break	Lobby, G/F
TADF and RISC I **Session Chair:** ***Howe-siang Tan (Nanyang Technological University)***		
11:15-11:45	Invited Talk#04: "Highly Efficient Organic Light Emitting Diodes Based on Thermally Activated Delayed Fluorescence" Chihaya Adachi (Kyushu University)	IAS Lecture Theater, G/F
11:45-12:15	Invited Talk#05: "Effect of Singlet Triplet Recycling in the Charge Transfer State Manifold and Molecular Geometry on Thermally Activated Delayed Fluorescence" Andy Monkman (University of Durham)	
12:15-12:30	General Talk#06: "How the Emitter-host Conformational and Electronic Interaction Can Determine TADF Performance" David Graves (University of Durham)	
12:30-14:00	Lunch at China Garden Restaurant, G/F, HKUST (For registered participants only)	

2D Electronic Spectroscopy
Session Chair: ***Andy Monkman (University of Durham)***

14:00-14:30	Invited Talk#07: "Ultrafast Multi-dimensional Electronic Spectroscopy and Its Applications to the Study of Light Harvesting Complexes" Howe-siang Tan (Nanyang Technological University)	IAS Lecture Theater, G/F
14:30-15:00	Invited Talk#08: "Coherent Charge Transfer in Organic Photovoltaics Probed by Ultrafast Spectroscopies" Margherita Maiuri (Princeton University)	
15:00-15:30	Invited Talk#09: "Two-dimensional Photocurrent Excitation Coherence Spectroscopy in Polymer: Fullerene Solar Cells" Carlos Silva (University of Montreal)	
15:30-16:00	Invited Talk#10: "Dielectric Effects in Photovoltaic Polymers" Franky So (University of Florida)	
16:00-16:30	Coffee break	Lobby, G/F

Exciton Fission/Fusion
Session Chair: ***Carlo Silva (University of Montreal)***

16:30-17:00	Invited Talk#11: "Charge Photogeneration in Donor-acceptor Blends Based on Low Band-gap π- conjugated Copolymers; the Effect of Singlet-fission" Valy Vardeny (The University of Utah)	IAS Lecture Theater, G/F
17:00-17:15	General Talk#12: "Triplet State Formation in Low-bandgap Polymer:Fullerene Photovoltaic Blends" Frédéric Laquai (Max Planck Institute for Polymer Research; King Abdullah University of Science and Technology)	
17:15-17:45	Invited Talk#13: "Ultrafast Vibrational Dynamics of Singlet Exciton Fission and Triplet Transfer to Inorganic Semiconductors" Akshay Rao (University of Cambridge)	

17:45-18:00	General Talk#14: "Triplet–Triplet Annihilation-Induced Up-Converted Delayed Luminescence in Solid-State Organic Composites: Monitoring Low-Energy Photon Up-Conversion at Low Temperatures" Panagiotis E Keivandis (Cyprus University of Technology)	
18:00-18:30	Invited Talk#15: "Emitting Dipole Orientation of Phosphorescent Dyes in OLEDs" Jang-joo Kim (Seoul National University)	
18:30-20:00	Conference Reception and Poster Session	Lobby, G/F

16 June 2015 (Tue) - Day 2

Time	Event	Venue
08:30-17:00	Conference Registration	Lobby, G/F
Single Molecule **Session Chair:** ***Akshay Rao (University of Cambridge)***		
09:00-09:45	Plenary Talk#16: "Chromophore Interactions in Conjugated Polymers" Lewis Rothberg (University of Rochester)	IAS Lecture Theater, G/F
09:45-10:15	Invited Talk#17: "Energy and Charge Transfer in Single Chain Conjugated Polymers and Oligomers" Kirk S Schanze (University of Florida)	
10:15-10:45	Invited Talk#18: "Molecular-level Study and Control of Conformation and Photophysics in Conjugated Molecular Complexes" Martin Vacha (Tokyo Institute of Technology)	
10:45-11:15	Coffee break	Lobby, G/F
OLED and Light Emitting Materials I **Session Chair:** ***Lewis Rothberg (University of Rochester)***		
11:15-11:45	Invited Talk#19: "New Strategies Towards Design of Luminescent Metal-Ligand Chromophoric Ensembles, Conjugates and Nano-Assemblies for Sensing and Bioassays" Vivian Wing-Wah Yam (The University of Hong Kong)	IAS Lecture Theater, G/F
11:45-12:15	Invited Talk#20: "Organic Nanoparticles for Sensing, Imaging and Therapy" Bin Liu (National University of Singapore)	
12:15-12:30	General Talk#21: "Hetero Triplet Fusion in Acene-Based Organic Light-Emitting Diodes" Marc Etherington (University of Durham)	
12:30-12:45	General Talk#22: "The Effect of Exciplex Formation on the Performance of Organic Light Emitting Diodes" Hameed A Al Attar (University of Durham)	

12:45-14:15	Lunch at China Garden Restaurant, G/F, HKUST (For registered participants only)	

Organic and Hybrid (Perovskite) Solar Cells I
Session Chair: ***Jiannong Wang (The Hong Kong University of Science and Technology)***

14:15-14:45	Invited Talk#23: "Photophysical Versus Structural Properties in Hybrid Lead-Halide Perovskites" Annamaria Petrozza (Istituto Italiano di Tecnologia)	IAS Lecture Theater, G/F
14:45-15:15	Invited Talk#24: "Interfacial Exciton Dissociation at Metal/Organic Interface in Organic Solar Cells " Furong Zhu (Hong Kong Baptist University)	
15:15-15:30	General Talk#25: "Small-Molecule Cathode Interfacial Material Based on Phenanthroline Derivative for High-Performance Organic Photovoltaics" Xuhui Zhu (South China University of Technology)	
15:30-15:45	General Talk#26: "Probing the Ultrafast Vibronic Dynamics of Charge Transfer in Organic Photovoltaic Blends" Andreas C Jakowetz (University of Cambridge)	
15:45-16:15	Invited Talk#27: "From Engineering Interfaces in Soft Electronic Materials to Efficient Perovskite Photovoltaics" Sergei Tretiak (Los Alamos National Laboratory)	
16:15-16:45	Coffee break	Lobby, G/F

Spin and Magnetic Field Effect
Session Chair: ***Martin Vacha (Tokyo Institute of Technology)***

16:45-17:15	Invited Talk#28: "Magnetic Field Effect in Organic Semiconductor Devices" Jiannong Wang (The Hong Kong University of Science and Technology)	IAS Lecture Theater, G/F
17:15-17:30	General Talk#29: "High Field Magneto-luminescence in Organic Semiconductors" Eitan Ehrenfreund (Technion-Israel Institute of Technology)	

17:30-18:00	Invited Talk#30: "Spontaneous Spin Polarization in Charged and Excited Organic Molecules" Shijie Xie (Shandong University)
18:00-18:30	Invited Talk#31: "Photothermoelectric Effect of Organic Semiconductors in Enabling NIR Detection" Chongan Di (Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences)
18:30-18:45	General Talk#32: "Molecular Dynamics Simulations of the Conformational Effects on Optoelectronic Phenomena in Conjugated Semiconducting Oligomers" Jack Wildman (Heriot-Watt University)
18:45-19:00	Short break (Coach departs at 19:00 for Conference Banquet)
19:00-21:30	Conference Banquet at Sai Kung (For registered participants only)

17 June 2015 (Wed) - Day 3

Time	Event	Venue
08:30-12:00	Conference Registration	Lobby, G/F
Optical and Ultrafast Spectroscopy I **Session Chair:** ***Valy Vardeny (The University of Utah)***		
09:00-09:45	Plenary Talk#33: "Controlling Cell Functions by Light" Guglielmo Lanzani (Istituto Italiano di Tecnologia and Politecnico di Milano)	IAS Lecture Theater, G/F
09:45-10:15	Invited Talk#34: "Developing Advanced Structural Probes to Identify the Dominant Optical Transitions in Donor-Acceptor Copolymers and Their Impact on Photostability" Ji-seon Kim (Imperial College London)	
10:15-10:30	General Talk#35: "Optical Vibrational Control of Charge Transport in Organic Semiconductors" Artem A Bakulin (University of Cambridge)	
10:30-10:45	General Talk#36: "Spontaneous Fluctuation of Transition Dipoles Revealed by Single-molecule Spectroscopy" Florian Steiner (University of Regensburg)	
10:45-11:15	Coffee break	Lobby, G/F
Carrier Dynamic and Energy Relaxation **Session Chair:** ***Annamaria Petrozza (Istituto Italiano di Tecnologia)***		
11:15-11:45	Invited Talk#37: "Decoherence and Energy Relaxation within Charge Transport Process in Crystalline Organic Semiconductors" Changqin Wu (Fudan University)	IAS Lecture Theater, G/F
11:45-12:00	General Talk#38: "Tracking Charge Photogeneration in 3-phase Polymer:Fullerene Blends" Justin Hodgkiss (Victoria University of Wellington; MacDiarmid Institute for Advanced Materials and Nanotechnology)	
12:00-12:15	General Talk#39: "Charge-transfer Dynamics and Vibrational Coherence in Polymer/Fullerene Blends" Yin Song (University of Toronto)	

12:15-12:45	Invited Talk#40: "Time-dependent Wavepacket Diffusive Method and Its Applications to Carrier Quantum Dynamics in Organic Materials" Yi Zhao (Xiamen University)
12:45-14:00	Lunch at China Garden Restaurant, G/F, HKUST (For registered participants only)
14:10-14:30	Coach from China Garden Restaurant to HKUST Pier (Boat departs at 14:30)
14:30-18:30	Half-day Boat Tour (For registered participants only)

18 June 2015 (Thu) - Day 4

Time	Event	Venue
TADF and RISC II Session Chair: *Zhigang Shuai (Tsinghua University)*		
09:00-09:45	Plenary Talk#41: "RISC from High-lying Triplet to Singlet: Optical Probes and Application for OLEDs" Yuguang Ma (South China University of Technology)	IAS Lecture Theater, G/F
09:45-10:00	General Talk#42: "Tailored Polymers for Efficient Thermal Activated Delayed Fluorescence. Towards Printable TADF OLEDs" Fernando B Dias (University of Durham)	
10:00-10:30	Invited Talk#43: "Utilizing the Doublet Emission of Neutral π-radical to Break the 25% Upper Limit of Internal Quantum Efficiency of OLEDs" Feng Li (Jilin University)	
10:30-10:45	General Talk#44: "Exciplex Way From Blue to Red, Novel TADF Emitters" Przemyslaw Data (University of Durham)	
10:45-11:15	Coffee break	Lobby, G/F
OLED and Light Emitting Materials II Session Chair: *Patrick Parkinson (University of Manchester)*		
11:15-11:45	Invited Talk#45: "Modeling Aggregation Effects on Molecular Light-emitting Quantum Efficiency and Spectroscopy" Zhigang Shuai (Tsinghua University)	IAS Lecture Theater, G/F
11:45-12:00	General Talk#46: "The Optical Properties of Conjugated Materials and their Aggregates: Towards Imaging of Films and Devices" Linda Peteanu (Carnegie Mellon University)	
12:00-12:30	Invited Talk#47: "Highly Solid-State Emissive Organic Fluorescent Materials" Wenjing Tian (Jilin University)	
12:30-14:00	Lunch at China Garden Restaurant, G/F, HKUST (For registered participants only)	

Organic and Hybrid (Perovskite) Solar Cells II
Session Chair: ***Kok Wai Cheah (Hong Kong Baptist University)***

14:00-14:30	Invited Talk#48: "Putting Organic and Organic/Inorganic Hybrid Materials to Work for Efficient Solar Energy Conversion" Shihe Yang (The Hong Kong University of Science and Technology)	IAS Lecture Theater, G/F
14:30-14:45	General Talk#49: "Modulating Electron - Hole Interaction in a Hybrid Lead Halide Perovskite with Electric Field" Ajay Ram Srimath Kandada (Istituto Italiano di Tecnologia)	
14:45-15:15	Invited Talk#50: "Comprehensive Studies of New Schemes for Enhancing the Carrier Extraction and Light Absorption of Organic/Inorganic Solar Cells" Wallace C H Choy (The University of Hong Kong)	
15:15-15:30	General Talk#51: "Impact of Solvent Additive on Transport Properties and Photovoltaic Performance in Polymer:Fullerene Bulk-heterojunction System" Shu Kong So (Hong Kong Baptist University)	
15:30-16:00	Invited Talk#52: "Multi-scale Modeling of Electronic Processes at the DTDCTB/C_{60} Interfaces for Organic Photovoltaics" Yuanping Yi (Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences)	
16:00-16:30	Coffee break	Lobby, G/F

Optical and Ultrafast Spectroscopy II
Session Chair: ***Shihe Yang (The Hong Kong University of Science and Technology)***

16:30-17:00	Invited Talk#53: "Ultrafast Energy Dynamics in Biomimetic Nanoring Complexes" Patrick Parkinson (University of Manchester)	IAS Lecture Theater, G/F
17:00-17:15	General Talk#54: "Ultrafast Broadband Photoluminescence Spectroscopy for Advanced Optoelectronic Materials" Kai Chen (Victoria University of Wellington; MacDiarmid Institute for Advanced Materials and Nanotechnology)	

17:15-17:30	General Talk#55: "Structure-Directed Exciton Dynamics in Templated Porphyrin Nanorings" Juliane Gong (University of Oxford)
17:30-18:00	Invited Talk#56: "Emerging Organic Optoelectronics Devices" Kok Wai Cheah (Hong Kong Baptist University)
18:00-18:15	General Talk#57: "Multi-Molecular Conical Intersections in Ultrafast Singlet Exciton Fission" Andrew J Musser (University of Cambridge)
18:15-18:30	General Talk#58: "Optically-pumped Lasing and Hot Phonon Bottleneck in Mixed Halide Perovskite Photovoltaic Semiconductors" Felix Deschler (University of Cambridge)

19 June 2015 (Fri) - Day 5

Time	Event	Venue
Organic and Hybrid (Perovskite) Solar Cells III **Session Chair:** ***Charles Surya (The Hong Kong Polytechnic University)***		
09:00-09:30	Invited Talk#59: "Aggregation and Morphology Control Enables Multiple Cases of High-efficiency Polymer Solar Cells" He Yan (The Hong Kong University of Science and Technology)	IAS Lecture Theater, G/F
09:30-10:00	Invited Talk#60: "A Multiscale Simulation Framework for Novel Photovoltaic Materials" Lingyi Meng (Xiamen University)	
10:00-10:15	General Talk#61: "Mapping Photoinduced Ionic Migration and Segregation in Mixed-halide Hybrid Perovskites" Alex J Barker (Istituto Italiano di Tecnologia)	
10:15-10:30	General Talk#62: "Bimolecular Nature of Fluence Dependent Radiative Recombination Processes in Hybrid Lead Bromide and Iodide Perovskites" Johannes M Richter (University of Cambridge)	
10:30-11:00	Coffee break	Lobby, G/F
Organic and Hybrid (Perovskite) Solar Cells IV **Session Chair:** ***Kam Sing Wong (The Hong Kong University of Science and Technology)***		
11:00-11:30	Invited Talk#63: "Defect Engineering and the Enhancement of The Power Conversion Efficiency of Perovskite based Solar Cells" Charles Surya (The Hong Kong Polytechnic University)	IAS Lecture Theater, G/F
11:30-11:45	General Talk#64: "Local Versus Long-Range Diffusion Effects of Photoexcited States on Radiative Recombination in Organic-Inorganic Lead Halide Perovskites" Milan Vrućinić (University of Cambridge)	
11:45-12:00	General Talk#65: "Photoconductive Cathode Interlayer for Highly Efficient Inverted Polymer Solar Cells" Zengqi Xie (South China University of Technology)	

12:00-12:15	General Talk#66: "Anisotropic Carrier Thermalisation and Morphology-dependent Polarisation Memory in Organometallic Halide Perovskites" Jasmine Rivett (University of Cambridge)
12:15-12:30	Conference Closing
12:30-14:00	Lunch at China Garden Restaurant, G/F, HKUST (For registered participants only)

List of Posters

Poster No.	Title and Author
P01	Poster#01: "Luminescence Enhancement in Dinuclear Alkynylplatinum(II) Complexes Driven by Hierarchical Assembly Through Pt···Pt and π–π Stacking Interactions" Sammual Yu Lut Leung (The University of Hong Kong)
P02	Poster#02: "Synthesis and Photo-Induced Electron Injection Process Studies in a Ruthenium Containing Triblock Copolymer/Multi-Walled Carbon Nanotubes Composite" Lili Du (The University of Hong Kong)
P03	Poster#03: "Twisting Donor-acceptor-donor Type Pyridine Derivatives: The Synthesis and Photophysical Investigations of Intramolecular Charge Transfer State" Murat Aydemir (University of Durham)
P04	Poster#04: "Realization of the Population Inversion in a Conjugated Polymer by a Single or Double Stimulating Pulse" Kun Gao (Shandong University)
P05	Poster#05: "Tuning the Singlet–triplet Energy Gap of AIE Luminogens: Crystallization-induced Room Temperature Phosphorescence and Delay Fluorescence, Tunable Temperature Response, Highly Efficient Non-doped OLEDs" Yilin Zhang (The Hong Kong University of Science and Technology)
P06	Poster#06: "Two-photon Optical Properties of AIE-active D-TPE-A Molecules: Aggregation Enhancement and Structure-Property Relationships" Yilin Zhang (The Hong Kong University of Science and Technology)
P07	Poster#07: "Spectroscopic Studies of Different Poly3hexylthiophene Chain Environments in a Polyfluorene Matrix" Paloma Santos (University of Durham)
P08	Poster#08: "Using Resonance Raman Scattering and Isotopic Substitution Techniques to Probe AIE Process from Theoretical Insight" Tian Zhang (Tsinghua University)

Poster No.	Title and Author
P09	Poster#09: "Tuning of Intramolecular Charge Transfer Reactions in Dipolar Pyrrolo-pyrimidine Derivatives and Their Fluorescence Sensing Properties" Saulius Jursenas (Vilnius University)
P10	Poster#10: "Tuning the Optical Properties of Dipolar Derivatives of 1,8-Naphthalimide: Effects of the Substituents and the Environment" Saulius Jursenas (Vilnius University)
P11	Poster#11: "Light-emitting Polycyclic Aromatic Hydrocarbon Synthesized by Regioselective Photocyclization and Its Application in Optical Waveguide" Xinggui Gu (The Hong Kong University of Science and Technology)
P12	Poster#12: "Bipolar Gold(III) Complexes for Solution-Processable Organic Light-Emitting Devices with a Small Efficiency Roll-Off" Man Chung Tang (The University of Hong Kong)
P13	Poster#13: "Emission Mechanisms and Applications of Phenylbenzoxales Based AIE Compounds" Yan Qian (Nanjing University of Posts and Telecommunications)
P14	Poster#14: "Material Selection for Donor Materials in Small Molecular-Based Bulk Heterojunction Organic Photovoltaic Devices" Evans Yi Chun Wong (The University of Hong Kong)
P15	Poster#15: "Singlet Fission in Mixed Films of Pentacene and Perfluoropentacene" Vincent Kim (University of Cambridge)
P16	Poster#16: "Excited State Transitions of the Emissive Intramolecular Charge-transfer States in Thermally Activated Delayed Fluorescence Molecules" Marc K Etherington (University of Durham)
P17	Poster#17: "The Influences of Host Matrix and D-A Molecular Geometry on Thermal Assisted Delayed Fluorescence and Device Performance" Roberto S Nobuyasu (University of Durham)

Poster No.	Title and Author
P18	Poster#18: "Development of Pure Organic Materials with Long-Lived and Efficient Room Temperature Phosphorescence" Weijun Zhao (The Hong Kong University of Science and Technology)
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P27	Poster#27: "Plasmonic-Electrical Effect on Organic Solar Cell by the Incorporation of Metallic Nanostructures" Wallace C H Choy (The University of Hong Kong)
P28	Poster#28: "Plasmonic-Electrical Effects in Metal Oxide Transport Layers for High-Performance Organic Photovoltaics" Di Zhang (The University of Hong Kong)
P29	Poster#29: "Morphology Enhancement in $CH_3NH_3PbI_3$ Perovskite Films through Vacuum-Assisted Thermal Annealing" Fengxian Xie (The University of Hong Kong)
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P31	Poster#31: "High-efficiency Non-fullerene Organic Solar Cells Enabled by a Difluorobenzothiadiazole-based Donor Polymer Combined with a Properly Matched Small Molecule Acceptor" Jingbo Zhao (The Hong Kong University of Science and Technology)
P32	Poster#32: "Low Threshold Lasing and Optical Properties of Vacuum-Assisted Thermal Annealed Perovskite Thin Films" Hexiang He (The Hong Kong University of Science and Technology)
P33	Poster#33: "Photophysical Characterization of Red Emitters for Solution-Processed Small-Molecule OLEDs and Organic Photovoltaic Devices" Flavio Franchello (University of Durham)
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Poster No.	Title and Author
P36	Poster#36: "Broadband Light Absorption Enhancement in Moth’s Eye Nanostructured Organic Solar Cells" Weixia Lan (Hong Kong Baptist University)
P37	Poster#37: "Efficient Organic-inorganic Hybrid Perovskite Solar Cells Fabricated under High Humidity Condition" Guijun Li (The Hong Kong University of Science and Technology)
P38	Poster#38: "An Insight on Oxide Interlayer in Organic Solar Cells: From Light Absorption and Charge Collection Perspectives" Zhenghui Wu (Hong Kong Baptist University)
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Abstracts

[Talk#01]

Molecular Metamaterials: Using Polymer Conformation to Define Photonic Nanostructures

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Metamaterials are a promising new class of materials in which sub-wavelength physical structures, rather than variations in chemical composition, can be used to modify the nature of their interaction with electromagnetic radiation. Traditionally, metamaterials have been constructed by structuring thin metal films into a variety of periodic designs that, for visible spectrum applications, are required to be of a few-nm dimensions and hence typically need electron-beam processing. We show that a metamaterials approach, using a discrete physical geometry (conformation) of the segments of poly(9,9-dioctylfluorene) (PFO) chains as the vector for a substantial refractive index change, can be used to enable visible wavelength, conjugated polymer photonic elements. In particular, we demonstrate that a novel form of dip-pen nanolithography provides an effective means to both structure and pattern the so-called β-phase conformation and that this can be done on length scales ≤ 500 nm, as required to fabricate a variety of photonic elements [1]. In addition, we discuss recent studies on the detailed nature of the β-phase and its dependence on chemical structure and processing conditions; solution crystallization and gelation studies provide additional insights [2].

References

[1] Perevedentsev A., Sonnefraud Y., Sharma S., Cass A.E.G., Maier S.A., Kim J.S., Stavrinou P.N., Bradley D.D.C., “Dip-pen patterning of poly(9,9-dioctylfluorene) chain-conformation-based nanophotonic elements”, *Nat. Commun.* 6 (2015), p 5977.

[2] Perevedentsev A., Fledman K., Stavrinou P.N., Bradley D.D.C., Smith P., “Solution-Crystallisation and Related Phenomena in 9,9-dialkyl-fluorene Polymers: I. Crystalline Polymer-Solvent Compound Formation for Poly(9,9-dioctylfluorene)” (2015), submitted; Perevedentsev A., Stavrinou P.N., Bradley D.D.C., Smith P., “Solution-Crystallisation and Related Phenomena in 9,9-dialkyl-fluorene Polymers: II. Influence of Side-Chain Structure” (2015), submitted.

[Talk#02]

Organic & Hybrid Photonic Crystals: From Lasers to Sensors

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In this communication, we review the opportunities provided by polymer PhC and we will focus on recent results obtained with 2D and 3D colloidal arrays (respectively, microsphere monolayers and opals) as well as on 1D all-polymer structures, which may join to photonic functionalities mechanical flexibility in free-standing systems, i.e. properties unprecedented for their inorganic counterpart.
1D all-polymer photonic crystals (i.e. Distributed Bragg Reflectors and microcavities) are grown by spin-coating by using polymer solutions in orthogonal solvents.[1, 2] Even though, the technique is very simple, cheap and well known, limitations occur when different constraints, such as high dielectric contrast, solvent orthogonality, control of the interfaces and layer thickness, transparency, lack of light scattering, have to be simultaneously considered. In spite of that, the technique allows to prepare free-standing, flexible and high optical quality DBR and microcavities (Q ~ 250), which can be successfully doped with photoactive materials (semiconducting, photochromic and porous polymers, J-aggregates) to obtain photonic platforms suitable for lasing, switching and sensing.[1-5]
2D PhC, i.e. microsphere arrays can be prepared by floating or spin-coating.[6] Such systems have been successfully used as a template for grazing incident gold evaporation thus generating nanocrescents possessing different kind of anisotropic plasmonic resonances. When gold nanocrescents are grown on the opal surface, interactions between selected plasmonic resonances and photonic modes can be observed.[6] Moreover, microsphere monolayers cover with metallic nanocrescents show unusual second harmonic generation of circular dichroism.[7]
Finally, different chemical and physical methods have been used to embed fluorescent conjugated systems into opals, the well-known playground for 3D photonic crystals. The photophysics of such PhC is investigated in order to assess fluorescence enhancement effects and modulation of the radiative lifetime.[8-11]

References

[1] L. Frezza et al., “Directional Enhancement of Spontaneous Emission in Polymer Flexible Microcavities”, *J. Phys. Chem. C,* 115, (2011), 19939-19946.
[2] G. Canazza et al.,”Lasing action from all polymer microcavities”, *Laser Phys. Lett.* 11, (2014), 035804.
[3] S. Pirotta et al.,”Strong coupling between excitons in organic semiconductors and Bloch surface waves”, *Appl. Phys. Lett.*, 104, (2014), 051111.
[4] L. Fornasari, F. Floris, M. Patrini, G. Canazza, G. Guizzetti, D. Comoretto and F. Marabelli, “Fluorescence excitation enhancement by Bloch surface wave in all-polymer one-dimensional photonic structure”, *Appl. Phys. Lett.* 105, (2014), 053303.
[5] P. Lova et al., “Polymer distributed Bragg reflectors for vapor sensing”, *ACS Photonics,* submitted.
[6] V. Robbiano et al., “Hybrid plasmonic-photonic nanostructures: gold nanocrescents over opals”, *Adv. Optical Mater.* 1, (2013), 389-396.
[7] A. Belardini et al., “Second harmonic generation circular dichroism from self-ordered hybrid plasmonic-photonic metasurface”, *Adv. Optical Mater.* 2, (2014), 208-213.
[8] L. Berti et al., “Spectroscopic investigation of artificial opals infiltrated with a heteroaromatic quadrupolar dye”, *J. Phys. Chem. C*, 114, (2010), 2403-2413.
[9] F. Di Stasio et al., “Fluorescent polystyrene photonic crystals self-assembled with watersoluble conjugated polyrotaxanes”, *APL Materials* 1, (2013), 042116.
[10]K. Sparnacci et al., “Preparation, properties and self-assembly behaviour of PTFE-based core-shell nanospheres”, *J. Nanomater.* 2012, (2012), 980541.
[11]S.V. Radice et al., “Photonic Crystals”, *Int. Appl. Patent N.* PCT/EP2014/055590, 02.10.2014.

[Talk#03]

Optical Gain Property Investigation of Novel Green-yellow Emission Polymer F8F5BT and Its Blends with PFO

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Semiconducting conjugated polymers have received considerable interest as promising solid-state gain media for lasers and amplifiers. Optically pumped polymer lasers have been demonstrated across the full visible spectrum. Efforts are consequently being made to lower lasing thresholds in order to make progress towards an inorganic laser diode pumped or electrically pumped polymer laser. Here, we report a study of the optical gain properties of our newly developed green-yellow emission polymer gain media F5F8BT and its blends with fluorene-based copolymers, PFO. F8F5BT and blends comprising 5% - 20% F5F8BT and 95% - 80% PFO show amplified spontaneous emission (ASE) in the range 550 - 570 nm with very low pump energy requirements (~ 80 nJ, 550 μm × 4 mm excitation stripe, 5 ns pulse, 10 Hz). Although F5F8BT and F8BT demonstrate similar photoluminescence quantum efficiency (PLQE) and ASE characters, the output-input characters evidence that the introduction of F5 to the F8BT polymer lead to a higher slope efficiency from F8F5BT/PFO film than from F8BT/PFO film. The output characteristics of ASE will be discussed in detail, including the influence of the chemical structure, molecular weight, film morphology and the blend composition.

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References

[1] R. Xia, P. N. Stavrinou, D. D. C. Bradley, and Y. Kim, “Efficient optical gain media comprising binary blends of poly(3-hexylthiophene) and poly(9,9-dioctylfluorene-co-benzothiadiazole)”, *J of Applied Physics,* Vol. 111, (2012), P123107.

[2] B. Yap, R Xia, M. Campoy-Quiles, P. N. Stavrinou and D. D. C. Bradley, “Simultaneous Optimization of Semiconducting Polymer Films for Optical Gain and Charge Carrier Mobility”, *Natural Materials*, Vol. 7, (2008), pp376-380.

[3] R. Xia, G. Heliotis, P. N. Stavrinou and D. D. C. Bradley, “Polyfluorene distributed feedback lasers operating in the green-yellow spectral region”, *Applied Physics Letters,* Vol. 87, (2005), P031104.

[Talk#04]

Highly Efficient Organic Light Emitting Diodes Based on Thermally Activated Delayed Fluorescence

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Organic compounds that exhibit high efficiency are required to realize inexpensive organic light-emitting diodes (OLEDs) for future displays and lighting applications. Here we mention the design rules for increasing the electroluminescence efficiency of organic molecules that exhibit thermally activated delayed fluorescence (TADF). We show that a large delocalization of the highest occupied molecular orbital and lowest unoccupied molecular orbital in these charge transfer compounds enhances the rate of radiative decay considerably by inducing a large oscillator strength even when there is a small overlap between the two wavefunctions. A compound based on our design principles exhibited a high rate of fluorescence decay and efficient up-conversion of triplet excitons into singlet excited states, leading to both photoluminescence and internal electroluminescence quantum yields of nearly 100%.

Further, we demonstrate a novel pathway for highly-efficient fluorescence-based OLEDs by exploiting TADF through the use of an assistant dopant. In the system, triplet excitons created on a TADF molecule by electrical excitation are up-converted to the singlet state, and the singlet excitons are completely transferred to the singlet state of a fluorescent emitter molecule *via* a Förster energy transfer process, which results in efficient radiative decay from the singlet state of the fluorescent emitter. The OLEDs with TADF assistant dopants showed high external EL quantum efficiencies of 13.4 - 18.0% for blue, green, yellow, and red emission, indicating that the exciton production efficiency reached nearly 100%. We named this energy transfer process from TADF molecules to fluorescent emitters "TADF-assisted fluorescence (TAF)". In addition, the enhancement of operational stability compared to that of OLEDs using the TADF molecules as emitters was observed for the TAF-OLEDs, indicating that the TAF process can provide dual enhancement of both EL efficiency and operational stability in OLEDs by rapid upconversion of triplet excitons.

References

[1] H. Uoyama, et.al., "Highly efficient organic light-emitting diodes from delayed fluorescence", *Nature*, **492**, pp234-238, (2012).
[2] H. Nakanotani, et.al., "High efficiency organic light-emitting diodes with fluorescent emitters", *Nat. Commun*, **5**, No.4016, (2014).

[Talk#05]

Effect of Singlet Triplet Recycling in the Charge Transfer State Manifold and Molecular Geometry on Thermally Activated Delayed Fluorescence

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For specific donor acceptor molecular configurations, the CT singlet and triplet states are found to be the lowest lying excited states of the molecule with very small electron exchange energies < kT. In these cases the decay kinetics of the molecules become significantly different to normal molecules, and the effect of rapid recycling between CT singlet and triplet states is seen to greatly extend the lifetime of the ‘excited state’ and yield non-exponential decay. Quantum yields increase markedly, even though the intersystem crossing rate is fast, $> 10^7\ s^{-1}$. The decay kinetics is found to be very sensitive to both temperature and sample inhomogeneity[2]. Temperature dependent delayed emission measurements reveal very different time domain behaviour and the effects of ICT emitter inhomogeneity is revealed. Clear evidence will be given to show that TADF reaches 100% efficiency at harvesting triplet states[1], and device having > 15% EQE discussed.

We will show the results for an ICT molecule with highly controlled structure i.e. the donor and acceptor fragments are held rigidly orthogonal. In this molecule the CT states can clearly be seen to be the lowest energy states of the molecule with a very small exchange energy (singlet triplet gap). Here we find that there are substantial differences between optical and electroluminescent photophysics resulting in device being far more efficient than is suggested by the molecules PLQY. For the first time we can show that the PLQY of the emitter is not the figure of merit to use in a device, because the excited states are formed in a different way within the device which avoids a major excited state quenching mechanism. This will be discussed in a new molecule that has a PLQY of 30% but gives devices having >19% EQE.

References

[1] V. Jankus, C. J. Chiang, F. Dias, and A. P. Monkman, Adv Mater **25**, 1455 (2013).
[2] F. B. Dias, et al, Adv Mater **25**, 3707 (2013).
[3] V. Jankus, et al, Advanced Functional Materials **24**, 6178. (2014).

[Talk#06]

How the Emitter-host Conformational and Electronic Interaction Can Determine TADF Performance

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Thermally activated delayed fluorescence, herein known as TADF, has great potential for creating low cost and highly efficient organic light emitting diodes. Utilising intra-molecular charge transfer (ICT) states many different TADF molecules have been synthesised with varying degrees of success, but much is still unknown about the charge transfer state. It is hoped that a more thorough understanding of its underlying nature will yield further progress in this field.

In this presentation the model molecule “2d” is dispersed into various host matrices, and extensively characterised by photophysics methods [1]. It is clearly shown that high molecular triplet energy by itself is insufficient for creating a suitable host for a TADF emitter. Strong conformational and electronic emitter-host interactions are observed and it is shown that the charge transfer state is very sensitive to such manipulation. Depending on the choice of host material exciplex [2], intra-molecular charge transfer, ‘prompt’ excitonic or systems with delayed fluorescence through triplet triplet-triplet annihilation could come to dominate. Such triplet-triplet annihilation has been observed even milliseconds after excitation.

For future design of TADF emitting *systems* and devices it is imperative to not think of just the emitter molecule in isolation, or of excited species in terms of “pure” excited states. Clear guidelines for the creation of future efficient TADF systems are given.

References

[1] Graves D., Monkman A., “*How the emitter-host conformational and electronic interaction can determine TADF performance”*, not yet submitted as of 17th April 2015.
[2] Jankus V., Data P., Graves D., McGuiness C., Santos J., Bryce M.R., Dias F.B., Monkman A.P., “Highly Efficient TADF OLEDs: How the Emitter–Host Interaction Controls Both the Excited State Species and Electrical Properties of the Devices to Achieve Near 100% Triplet Harvesting and High Efficiency”, *Advanced Functional Materials*, 24, 39, (2014).

[Talk#07]

Ultrafast Multi-dimensional Electronic Spectroscopy and Its Applications to the Study of Light Harvesting Complexes

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Recently, there has been much interest in the application of ultrafast multi-dimensional electronic spectroscopy to the study of Light Harvesting Complexes [1]. We will review the basic principles of multi-dimensional electronic spectroscopy.

We report on our application of ultrafast two-dimensional (2D) and three-dimensional (3D) spectroscopies [2,3] to the study of the excitonic energy transfer (EET) processes of LHC II light harvesting complexes [4]. The EET process in light harvesting complexes is typically complex and proceeds in a multistep fashion. In 2DES, the spectra are presented in two frequency dimensions: one excitation frequency and one of the emission frequency. The crosspeaks on the 2D spectra correlates the donor exciton to the acceptor exciton. As this is a two point correlation, multistep processes can only be indirectly observed. In 3DES, with an additional frequency axis, three-step processes can be directly observed. A crosspeak on a 3D spectrum at (ω_a , ω_b , ω_c) will denote exciton a transferring energy to exciton c, via an intermediate exciton b. We have performed 3DES on LHCII trimers, and directly observed for the first time multistep EET process.

We also present recent results in our studies of the ultrafast dynamics of energy transfer from Chl b to Chl a band in trimeric and aggregated LHCII are examined using two-dimensional (2D) electronic spectroscopy. Global fitting analysis of the 2D spectra revealed similarities and differences between the kinetic components of LHCII trimers and aggregates. The 2D decay-associated spectra resulting from global analysis resolved an intermediate midenergy state of which the decay pathway depends on the physical state of LHCII.

References

[1] Schlau-Cohen GS, Ishizaki A, Fleming GR (2011) Chem. Phys. 386: 1–22.
[2] Zhang Z, Wells KL, Hyland EWJ, Tan HS (2012) Chem. Phys. Lett. 550: 156-161.
[3] Zhang Z, Wells KL, Tan HS (2012) Opt. Lett., 37: 5058-5060.
[4] Wells KL, Lambrev PH, Zhang Z, Garab G, Tan HS (2014) Phys. Chem. Chem. Phys. 16: 11640-11646.

[Talk#08]

Coherent Charge Transfer in Organic Photovoltaics Probed by Ultrafast Spectroscopies

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Photo-induced electron transfer from the photo-excited polymer donor to the fullerene acceptor is the cornerstone of the light-to-current conversion process in organic photovoltaic (OPV) devices [1, 2]. It is now accepted that this charge separation process occurs on an ultrafast (sub-100-fs) time scale. However, still very little is known about the initial quantum dynamics of the process in this class of technologically relevant material systems. Recently, few-optical-cycle pump-probe spectroscopy and two-dimensional electronic spectroscopy (2DES) have established themselves as powerful tools to probe the role of quantum coherence in the ultrafast charge transfer process [3, 4]. Here we use both techniques to unravel the primary photoinduced processes in P3HT:PCBM, which is a model all-organic donor/acceptor blend for OPV.

With high time resolution pump-probe spectroscopy, we have impulsively excited the polymer moiety with 8-fs pulses and probed the transient absorption on a broad spectral range, from 440 nm to 1400 nm [3]. Our experimental data show that excitons undergo an ultrafast dissociation in about 50 fs following excitation. By complementing the experimental results with time-dependent density functional theory (TDDFT) calculations we provide strong evidence on the role of vibronic coherence in the initial steps of the current photo-generation process. In particular the simulations show that strong vibronic coupling between electronic and nuclear degrees of freedom promotes delocalization of the photoexcited electronic wave packet across the interface. These results provide evidence for a coherent charge transfer mediated by strong vibronic coupling between polymer and fullerene.

The second part of the talk will present 2DES data on the same blend, acquired with a recently developed ultra-broadband apparatus [5]. These data support as well the key role the vibronic coherences in promoting the ultrafast electron transfer process in OPV blends.

References

[1] Brabec C. J., Zerza G., Cerullo G., De Silvestri S., Luzzati S., Hummelen J. C. and Sariciftci S., "Tracing photoinduced electron transfer process in conjugated polymer/fullerene bulk heterojunctions in real time," *Chemical Physics Letters* 340, (2001) 232-236.

[2] Guo J., Ohkita H., Benten H. and Ito S., "Charge Generation and Recombination Dynamics in Poly(3-hexylthiophene)/Fullerene Blend Films with Different Regioregularities and Morphologies," *Journal of the American Chemical Society* 132, (2010) 6154-6164.

[3] Falke S. M., Rozzi C. A., Brida D., Maiuri M., Amato M., Sommer E., De Sio A., Rubio A., Cerullo G., Molinari E. and C. Lienau, "Coherent ultrafast charge transfer in an organic photovoltaic blend," *Science* 344, (2014) 1001-1005.

[4] Song Y., Clafton S. N., Ryan D. Pensack, T. W. Kee and Scholes G. “Vibrational coherence probes the mechanism of ultrafast electron transfer in polymer–fullerene blends” *Nature Communication* 5, (2014) 4933-4940.

[5] Rèhault J., Maiuri M., Oriana A. and Cerullo G. “Two-dimensional electronic spectroscopy with birefringent wedges” *Review of Scientific Intruments* 85, (2014) 123107-17.

[Talk#09]

Two-dimensional Photocurrent Excitation Coherence Spectroscopy in Polymer: Fullerene Solar Cells

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In solar cells that incorporate semiconductor polymers as electron donors and fullerene derivatives as acceptors, a number of reports based on ultrafast optical probes reveal that charges can be generated on timescales significantly faster than ~100 fs in certain solid-state microstructures [1]. Techniques that have been applied in these studies include variants of visible transient absorption and photoluminescence spectroscopy, terahertz spectroscopy, time-resolved infrared spectroscopy, and femtosecond stimulated Raman spectroscopy. These probes allow measurement of population dynamics of relevant photoexcitations (excitons, polarons) but do not reveal directly how these interact to produce photocarriers [2]. Here, we present a non-linear coherent spectroscopy, photocurrent-detected two-dimensional spectroscopy (2DPC), which is an ultrafast optical technique belonging to a family of 2D Fourier-domain spectroscopies that allows measurement of correlations between optical transitions induced by short optical pulses. In our implementation, spectral correlations are detected via the time-integrated photocurrent produced in a photovoltaic diode. Four collinear ultrashort laser pulses (10 fs, centered at 600 nm in our experimental setup) excite the semiconductor polymer in the solar cell, with a variable delay that is independently controlled between each pulse in the sequence. Each pulse separately excites a quantum wavepacket with spectral phase and amplitude imparted by that pulse, while the effect of the pulse sequence is to collectively excite multiple quantum coherences. Interferences between the various combinations of the wavepackets determine linear and non-linear contributions to the material optical response. The fourth-order signal terms of the detected photocurrent are read using phase-sensitive detection schemes with reference waveforms corresponding to a modulation of specific phase combinations of the four femtosecond excitation pulses. By scanning the time delay between the pulses 1 and 2, as well as that between pulses 3 and 4 (coherence times), at a fixed delay between pulses 2 and 3 (population waiting time), one measures a two-dimensional coherence decay function that is Fourier transformed to produce a 2D photocurrent correlation excitation spectrum. Measurement of such spectra at different population waiting times provides insight into the role of spectral correlations and state coherence in photocurrent generation in such complex functional materials. We focus on solar cells produced by blends of a common carbazole-thiophene-benzothiadiazole polymer, PCDTBT (the donor polymer), and PCBM (the fullerene acceptor), in which we analyse the dynamics of total photocurrent generation via the time evolution of diagonal and off-diagonal spectral correlations. We address the role of vibronic coherence as well as resonant tunnelling in charge separation pathways on ultrashort timescales [4].

References

[1] S. Few, J.M. Frostab and J. Nelson, “Models of charge pair generation in organic solar cells”, *Phys. Chem. Chem. Phys.* **17**, 2311-2325 (2015).

[2] F. Provencher, N. Bérubé, A.W. Parker, G.M. Greetham, M. Towrie, C. Hellmann, M. Côté, N. Stingelin, C. Silva and S.C. Hayes, “Direct observation of long-range charge separation at polymeric semiconductor heterojunctions” *Nat. Commun.* **5**, 4288 (2014) and references therein.

[3] P.F. Tekavec, G.A. Lott, and A.H. Marcus, “Fluorescence-detected two-dimensional electronic coherence spectroscopy by acousto-optic phase modulation” *J. Chem. Phys.* **127**, 214307 (2007).

[4] E.R. Bittner and C. Silva, “Noise-induced quantum coherence drives photocarrier generation dynamics at organic semiconductor heterojunctions” *Nat. Commun.* **5**, 3119 (2014).

[Talk#10]

Dielectric Effects in Photovoltaic Polymers

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Solution processable polymeric bulk heterojunction solar cells have drawn a lot of attention due to their potential for low cost roll-to-roll manufacturing. Typical polymer solar cells are made with blends consisting of a polymer donor and a fullerene acceptor. Compared with inorganic semiconductors, polymer semiconductors have significantly lower dielectric constants leading to a strong localization of the charge transfer (CT) states and an additional energy loss due to the strong exciton binding energy. It is therefore important to determine how the dielectric properties of the polymer-fullerene blends affect the energy loss in polymer solar cells. However, one of the challenges is to determine the so-called effective bandgap of a polymer-fullerene blend which is the difference of the highest occupied molecular orbital (HOMO) energy of the polymer donor and the lowest unoccupied molecular orbital (LUMO) energy of the fullerene acceptor.

In this talk, we will first describe how we used charge modulated electroabsorption spectroscopy (CMEAS) to measure the effective bandgap energy of a polymer-fullerene blend. Knowing the effective bandgap energy and the energy loss due to carrier recombination in a polymer solar cell, we can determine the additional energy loss due to dielectric effects. From our data, we found that the excess energy loss in a polymer solar cell is a strong function of the dielectric constant of the polymer blend. For polymer blends with low dielectric constants, the photo-voltage loss can be as large as 0.35 V. On the other hand, there is no voltage loss if the dielectric constant is close to 5, suggesting that these polymer solar cells behave like their inorganic counter-parts. We also found that the dielectric properties have a strong effect on delocalization of the CT states. These findings will enable chemists to design novel polymers to minimize the energy loss in a polymer solar cell.

[Talk#11]

Charge Photogeneration in Donor-acceptor Blends Based on Low Band-gap π- conjugated Copolymers; the Effect of Singlet-fission

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We have used both cw and fs transient spectroscopies for studying the optical properties and photoexcitations in several low band-gap π-conjugated copolymers (such as PTB7, for example) that have been used in organic photovoltaic (OPV) applications. Surprisingly we obtained two primary photoexcitations that are generated within ~150 fs (our time resolution). We identify them as singlet exciton (S_1) and triplet-triplet (^{1}TT) pair, respectively; the latter species is a precursor for singlet-fission into two individual triplet excitons. The singlet exciton has been considered to be the only primary photoexcitation in regular π-conjugated polymers, and is related with a transient absorption band that peaks at an energy value close to the exciton binding energy (~0.4 eV). The TT pair, however is a novel photoexcitation species in low band-gap π-conjugated copolymers. It has an absorption band close to that of isolated triplet exciton, and may readily dissociate into two individual triplet excitons at time of the order of few microseconds. Furthermore we used the technique of transient magneto-photoinduced absorption (t-MPA) to identify the primary photoexcitations. We found that the singlet excitons and TT-pairs show identical t-MPA(B) response (where b is the magnetic field strength), but opposite in sign. This shows that the photogenerated singlet excitons and TT-pairs are ‘magnetically correlated’. In addition, the existence of t-MPA also shows that the TT-pair is indeed composed of two spin-carrying species, and is thus not a simple singlet state.

We further studied the charge photogeneration in blends of donor-acceptor (D-A) of low band-gap π-conjugated copolymers and fullerene molecules. We found that the T-T pair easily dissociate into polaron pair and triplet exciton at the D-A interfaces. This finding may be one of the reasons for the obtained high power conversion efficiency in OPV devices based on low bandgap copolymers.

[Talk#12]

Triplet State Formation in Low-bandgap Polymer:Fullerene Photovoltaic Blends

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Triplet state formation has recently been identified as a potential loss channel in low-bandgap:fullerene solar cells. However, the precise mechanism of the triplet formation and its impact on the photovoltaic performance under solar illumination is still controversially discussed. Here, we report on triplet state formation in different low-bandgap polymer:fullerene photovoltaic blends studied by femto- to microsecond broadband Vis-NIR transient absorption (TA) spectroscopy in combination with sophisticated soft modeling data analyses techniques such as evolving factor analysis (EFA) and multivariate curve resolution with alternating least squares (MCR-ALS). As an example I will first show experiments done on the prototypic low-bandgap donor-acceptor copolymers PCPDTBT and its silicon-substituted analogue PSBTBT.[1] Broadband Vis-NIR TA experiments revealed that after exciton dissociation and free charge formation is completed, fast sub-nanosecond non-geminate recombination occurs and leads to a substantial population of the polymer's triplet state. The extent to which triplet states are formed depends on the initial concentration of free charges, which itself is controlled by the microstructure of the blend, especially in case of PCPDTBT:$PC_{60}BM$. Interestingly, PSBTBT:$PC_{70}BM$ blends showed a higher charge generation efficiency, but less triplet state formation at similar free charge carrier concentrations. This indicates that the solid-state morphology and interfacial structure of PSBTBT:PC70BM blends reduce non-geminate recombination and thus triplet state formation, leading to increased device performance compared to optimized PCPDTBT:PC60BM blends.[1] Based on these observations I will then show very recent results obtained on DPP-based donor polymers [2] and PBDTTT-C:fullerene blends,[3] in which we observe almost quantitative triplet state formation by non-geminate recombination of free charges on the ns timescale followed by annihilation of triplet states and recreation of charge carriers on the ns-µs timescale.

References

[1] Etzold F., Howard I.A., Forler N., Melnyk A., Andrienko D., Hansen M.R. and Laquai F., "Sub-ns Triplet State Formation by Non-Geminate Recombination in PSBTBT:$PC_{70}BM$ and PCPDTBT:$PC_{60}BM$ Organic Solar Cells", *Energy Environ. Sci.* (2015), DOI: 10.1039/C4EE03630A.

[2] Ochsmann J.R, Chandran D., Gehrig D.W., Anwar H., Madathil P.K., Lee K.-S. and Laquai F., "Triplet state formation in photovoltaic blends of DPP-type copolymers and $PC_{71}BM$", *Macromol. Rap. Commun.* (2015), DOI: 10.1002/marc.201400714.

[3] Gehrig D.W., Howard I.A. and Laquai F., "Charge carrier generation followed by triplet state formation, annihilation, and carrier recreation in PBDTTT-C:$PC_{60}BM$ photovoltaic blends", submitted.

[Talk#13]

Ultrafast Vibrational Dynamics of Singlet Exciton Fission and Triplet Transfer to Inorganic Semiconductors

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Singlet exciton fission is the process in organic semiconductors through which a spin-singlet exciton converts into a pair of spin-triplet excitons residing on different chromophores, entangled in an overall spin-zero state [1]. For some systems, singlet fission has been shown to occur on the 100 fs timescale and with a 200% yield, but the mechanism of this process remains uncertain. Here we study a model singlet fission system, TIPS-pentacene, using ultrafast vibronic spectroscopy. We observe that vibrational coherence in the initially photogenerated singlet state is transferred to the triplet state. These observations provide experimental evidence for singlet fission proceeding via a multi-molecular conical intersection between the singlet and triplet pair manifolds, emphasise the key role of vibronic coupling and result in an intuitive explanation for the high fission yield [2]. We further report the transfer of molecular spin triplet excitons, formed via fission, from organic to inorganic semiconductors [3]. This transfer process occurs on sub-ps timescales with efficiencies as high as 95%. This result opens up a new route to couple organic and inorganic semiconductors and offers a very promising method to overcome the Shockley-Queisser limit on the efficiency of single junction photovoltaics.

References

[1] Rao, A. et al. Exciton fission and charge generation via triplet excitons in pentacene/C60 bilayers. ***JACS*** 132, 12698-12703, (2010), 10.1021/ja1042462.

[2] Musser et.al. Evidence for conical intersection dynamics mediating ultrafast singlet exciton fission, ***Nature Physics*** 11, 352–357 (2015), doi:10.1038/nphys3241

[3] Tabachnyk, M. et al. Resonant energy transfer of triplet excitons from pentacene to PbSe nanocrystals. ***Nature Materials*** 13, 1033-1038, (2014), 10.1038/nmat4093

[Talk#14]

Triplet−Triplet Annihilation-Induced Up-Converted Delayed Luminescence in Solid-State Organic Composites: Monitoring Low-Energy Photon Up-Conversion at Low Temperatures

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Lately, the process of low-energy photon upconversion via triplet−triplet annihilation (TTA-UC) [1, 2] has received wide attention as an attractive method for enabling the management of light in a broad range of applications [3-5]. Despite the intensive research on the applicability of TTA-UC, the fundamental processes that govern the TTA-UC photophysics in solid state multicomponent systems have not been clarified. For instance the process of triplet energy migration has not been fully discussed and the nature of energetic traps in the TTA-UC composite systems has not been identified. Here we address these issues by performing temperature-dependent time-integrated and time-gated luminescence spectroscopic studies on the model photon up-converting solid composite comprising the (2,3,7,8,12,13,17,18-octaethyl-porphyrinato) Pt^{II} (PtOEP) sensitizer, mixed with the blue-light emitting 9,10 diphenyl anthracene (DPA) activator [6]. Atomic force microscopy imaging and photoluminescence (PL) spectra find that the concentration of DPA excimeric and PtOEP triplet dimer sites affect the TTA-UC PL intensity of DPA. The strength of intermolecular interactions in the DPA:PtOEP solid state system can be tuned by keeping the composite either in its binary or in its ternary form with the use of the optically inert matrix of polystyrene (PS). The occurrence of triplet energy migration is studied by temperature-dependent PL measurements; when lowering the temperature to 100 K, the DPA up-converted luminescence intensity increases by a factor of 3, and this is attributed to the increased energetic disorder [7] of the DPA excited states in the PS:DPA:PtOEP system.

References

[1] Baluschev S., Miteva T., Yakutkin V., Nelles G., Yasuda, A., Wegner G. "Up-Conversion Fluorescence: Noncoherent Excitation by Sunlight", *Phys. Rev. Lett.* 97, 14, (2006), 143903.

[2] Singh-Rachford T. N., Castellano F. N., "Photon Upconversion Based On Sensitized Triplet−Triplet Annihilation", *Coord. Chem. Rev.* 254, 21-22, (2010), pp 2560−2573.

[3] Wohnhaas C., Turshatov A., Mailänder V., Lorenz S., Baluschev S., Miteva T., Landfester K., "Annihilation Upconversion in Cells by Embedding the Dye System in Polymeric Nanocapsules", *Macromolecular Bioscience*, 11, 6, (2011), pp 772–778.

[4] Cheng Y. Y., Fueckel B., MacQueen R. W., Khoury T., Clady R. G. C. R., Schulze T. F., Ekins-Daukes N. J., Crossley M. J., Stannowski B., Lips K., Schmidt T. W., "Improving the Light-Harvesting of Amorphous Silicon Solar Cells With Photochemical Upconversion", *Energy Environ. Sci.* 5, 5, (2012), pp 6953−6959.

[5] Börjesson K., Dzebo D., Albinsson B., Moth-Poulsen K.,"Photon Upconversion Facilitated Molecular Solar Energy Storage" *J. Mater. Chem. A*, 1, 30, (2013), pp. 8521-8524.

[6] Goudarzi H. and Keivanidis P. E., "Triplet−Triplet Annihilation-Induced Up-Converted Delayed Luminescence in Solid-State Organic Composites: Monitoring Low-Energy Photon Up-Conversion at Low Temperatures", *J. Phys. Chem. C.*, 118, 26, (2014), pp 14256–14265.

[7] Hoffmann S. T., Koenen J.-M., Scherf U., Bauer I., Strohriegl P., Bässler H., Köhler A., "Triplet-Triplet Annihilation in a Series of Poly(p-phenylene) Derivatives", *J. Phys. Chem. B*, 115, 26, (2011) pp 8417−8423.

[Talk#15]

Emitting Dipole Orientation of Phosphorescent Dyes in OLEDs

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Phosphorescent iridium complexes have long been thought to have random orientation when doped in an emitting layer due to their octahedron structures. Recently, however, some heteroleptic iridium complexes which have the ancillary ligands of β-diketonate or picolate have been reported to have preferred orientation of emission dipoles along horizontal direction (parallel to substrates). The outcoupling efficiency of the emitted light from the horizontally oriented emitting dipoles in an OLED can reach 45% which is much higher than isotropically oriented transition dipoles.[1] However, the origin of the preferred emitting dipole orientation (EDO) and the factors influencing the orientation have not been studied much.

In this presentation we will report the recent findings on the emitting dipole orientation of phosphorescent dyes, which can be summarized as follows: (1) Heteroleptic iridium complexes are more likely to have preferred orientation in host materials than homoleptic iridium complexes. (2) Three mutually orthogonal triplet transition dipole moments along the directions from the iridium core to the three C^N ligands with 3-fold rotational symmetry in homoleptic iridium complexes reduces the preferred EDO to a specific direction, resulting in almost isotropic EDO in doped films. In contrast, heteroleptic iridium complexes have two nearly parallel triplet transition dipole moments along the directions from the iridium core to the two C^N ligands with 2-fold symmetry. Therefore, heteroleptic iridium complexes can have larger anisotropy of EDO than homoleptic iridium complexes if the molecules align themselves with respect to the substrate. (3) Tetramethylheptadionate (tmd) ancillary ligand results in higher horizontal EDO than acetylacetonate (acac). (4) There is a strong linear correlation between the orientation of the emitting dipoles in films and the orientation of the transition dipole moments against the C2 axis of the heteroleptic Ir complexes. (5) The EDO of the heteroleptic Ir-complex varies from horizontal to isotropic, or even to vertical direction depending on host molecules. (6) Aliphatic host molecules do not seem to induce preferred orientation of dopant molecules. (7) The preferred molecular orientation of the host molecules does not induce the preferred molecular orientation of the dopant molecules. (8) Intermolecular interaction between complex dopants and the aromatic rings in the host molecules induces preferred orientation of dopant molecules. (9) The preferred horizontal orientation of dopant emitting dipoles is due to the formation of planar-structure supra-molecular assemblies of host and dopant molecules. (10) The vertical EDO is induced when they interact repulsively during the film deposition to form non-linear binding geometry. [2-4]

References

[1] Sei-Yong Kim, Won-Ik Jeong, Christian Mayr, Yong-Seo Park, Kwon-Hyeon Kim, Jeong-Hwan Lee, Chang-Ki Moon, Wolfgang Brutting and Jang-Joo Kim, Advanced Functional Materials, 23, 3896 (2013)

[2] Kwon-Hyeon Kim, Sunghun Lee, Chang-Ki Moon, Sei-Yong Kim, Young-Seo Park, Jeong-Hwan Lee, Jin Woo Lee, June Huh, Youngmin You, Jang-Joo Kim, Nature Communications, 5, (2014), 4769

[3] Kwon-Hyeon Kim, Chang-Ki Moon, Jeong-Hwan Lee, Sei-Yong Kim and Jang-Joo Kim, Advanced Materials, 26, (2014), 3844

[4] Chang-Ki Moon, Kwon-Hyeon Kim, Jin Woo Lee, and Jang-Joo Kim, Chemistry of Materials, DOI: 10.1021/acs.chemmater.5b00469 (2015)

[Talk#16]

Chromophore Interactions in Conjugated Polymers

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Many potential applications of conjugated polymers rely on their emissive properties and these in turn depend on packing morphology [1-3]. The organization of the chromophores regulates both the facility of energy transfer and the introduction of interchain species such as excimers and polaron pairs. Interchain interactions tend to result in reduced luminescence relative to isolated chromophores. Indeed, much of conjugated polymer spectroscopy and photophysics can be rationalized with a two chromophore ("isolated" and "aggregated") model [4]. These ideas translate remarkably well to the study of single polymer chains and VandenBout *et.al* [5] surprised the community by showing that single high molecular weight chains of MEH-PPV (Poly-2-methoxy-5(2'-ethylhexoxy)phenylene vinylene) nominally representing hundreds of chromophores could display blinking behavior in their photoluminescence (PL) as if they were single sites. In further work by Huser *et.al.* [6], it was suggested that the degree to which this is the case depended on processing conditions that presumably control the degree of folding of the chain back on itself to form effectively aggregated sites.

We will present studies of single polymer chains of MEH-PPV that exhibit unusual phenomenology that cannot be explained by these previous pictures. In particular, we show that interactions with oxygen can *increase* photoluminescence efficiency and that nearly non-emissive chromophores are extremely important to the single chain photophysics. Because the lowest energy chromophores have much lower PL efficiency [4], if these are bleached so that they are no longer energy acceptors, the PL of chromophores that funnel into these can be "turned on". In single chain spectroscopy, this behavior is manifest as "flaring", dramatic PL intensity spikes, and we show that these are observed in the presence of oxygen. Moreover, deliberate selective photooxidation can substantially increase brightness and stability of the PL for the same reasons. We will report systematic studies of how single polymer chain PL is affected by varying degrees of self-aggregation. On the basis of our observations, we propose modifications to the traditional two chromophore picture and discuss their consequences.

References

[1] Nguyen, T.Q., Doan, V. and Schwartz, B.J., "Conjugated polymer aggregates in solution: Control of interchain interactions", *J. Chem. Phys.* 110, 8 (1999) pp. 4068-4078.
[2] Samuel, I.D.W., Rumbles, G. and Collison, C.J., "Efficient interchain photoluminescence in a high-electron-affinity conjugated polymer", *Phys. Rev. B* 52, 16 (1995) pp. 11573-11576.
[3] Spano, F.C., "Excitons in conjugated oligomer aggregates, films and crystals", *Ann. Rev. Phys. Chem.* 57 (2006) pp. 217-243.
[4] Collison, C.J., Rothberg, L.J., Treemaneekarn, V. and Li, Y., "Conformational effects on the photophysics of conjugated polymers: A two species model for MEH-PPV spectroscopy and dynamics", *Macromolecules* 34,7 (2001) pp. 2346-2352.
[5] VandenBout, D.A., Yip, W.T., Hu, D.H., Fu, D.K., Swager, T.M. and Barbara, P.F., "Discrete intensity jumps and intramolecular electronic energy transfer in the spectroscopy of single conjugated polymer molecules", *Science* 277, 5329 (1997) pp. 1074-1077.
[6] Huser, T., Yan, M. and Rothberg, L.J., "Single chain spectroscopy of conformational dependence of conjugated polymer photophysics", *Proc Natl. Acad. Sci* 97,21 (2000) pp. 11187-11191.

[Talk#17]

Energy and Charge Transfer in Single Chain Conjugated Polymers and Oligomers

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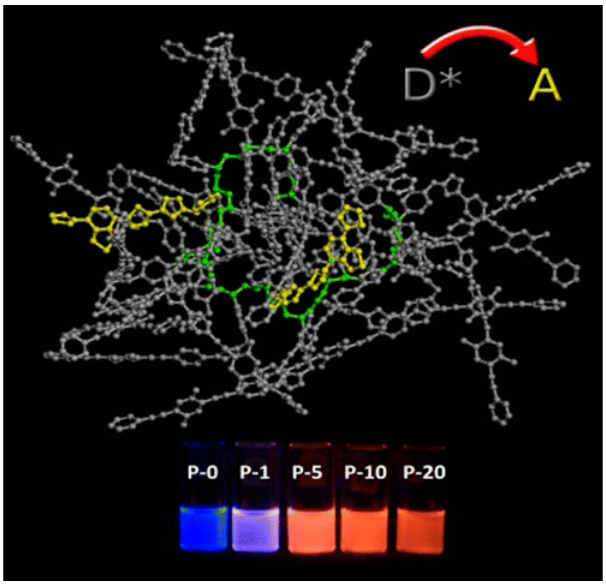
A series of main-chain conjugated and side-chain conjugated polymers that have been investigated to explore the dynamics of charge and energy transfer in isolated conjugated polymer chains. The assemblies include polystyrene based side-chain conjugated polymers, as well as poly(phenylene ethynylene) and poly(thiophene) main chain backbone structures. Energy transfer is investigated using low energy, highly fluorescent exciton traps while charge transfer is examined by using naphthalene diimide end-groups as electron acceptor. Dynamics of transport is examined by using ultrafast time resolved fluorescence and transient absorption spectroscopy.



References

[1] Keller, J. M.; McIlroy, S.; Sreearuothai, P.; Danilov, E. O.; Jiang, H.; Glusac, K. D.; Miller, J. R.; Schanze, K. S., "Negative Polaron and Triplet Exciton Diffusion in Organometallic "Molecular Wires", *J. Am. Chem. Soc.* **2011**, *133*, 11289-11298.

[2] Hsu, H.-Y.; Vella, J. H.; Myers, J. D.; Xue, J.; Schanze, K. S., "Triplet Exciton Diffusion in Platinum Polyyne Films", *J. Phys. Chem. B.* **2014**, *118*, 24282-24289.

[3] Chen, Z.; Grumstrup, E. M.; Gilligan, A. T.; Papanikolas, J. M.; Schanze, K. S., "Light Harvesting Polymers: Ultrafast Energy Transfer in Polystyrene Based Arrays of π-Conjugated Chromophores", *J. Phys. Chem. B* **2014**, *118*, 372-378.

[Talk#18]

Molecular-level Study and Control of Conformation and Photophysics in Conjugated Molecular Complexes

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Molecular-level understanding of collective photoresponse of conjugated molecular complexes is important both from the point of basic knowledge of the molecular photophysics as well as from the point of potential applications as photo-driven nanoscale devices. We study molecular complexes, either as assemblies composed of conjugated small molecules such as molecular aggregates, or as covalently linked chromophores such as conjugated polymers. Using different modes of electronic excitation, such as linear absorption, plasmonic near-field enhancement, energy transfer or charge recombination, we investigate the resulting excited state, the conformational states of the molecular complex and their cooperative dynamics. Further, we attempt to actively control the conformational state of the complexes by nanoscale mechanical manipulation using scanning probe microscopies [1] or other external stimuli. As one example, conformational changes of a conjugated polymer polyfluorene are studied on single-chain level upon excitation by linear absorption of light and by charge recombination. Both excitation mechanisms lead to dramatically different photophysical properties that reflect different intramolecular aggregation processes [2]. In photoluminescence the emission spectra are dominated by either singlet excitons or excimers formed via neutral ground-state aggregates. In electroluminescence the singlet exciton emission is absent and the spectra are either due to formation of charged ground-state aggregates or excimers. In both photoluminescence and electroluminescence thermally induced conformational dynamics of the polyfluorene chains leads to strong spectral dynamics on timescales of seconds. Further, as another example, we study the effect of polymer chain topology on the photophysical properties of conjugated polymers by comparing on single-molecule level the properties of cyclic and linear chains of poly(phenylene vinylene).

References

[1] Kobayashi H., Hirata S., Vacha M., “Mechanical Manipulation of Photophysical Properties of Single Conjugated Polymer Nanoparticles”, *J. Phys. Chem. Lett.* 4 (2013) 2591-2596

[2] Honmou Y., Hirata S., Komiyama H., Hiyoshi J., Kawauchi S., Iyoda T., Vacha M., “Single molecule electroluminescence and photoluminescence of polyfluorene unveils the photophysics behind the green emission band”, *Nature Commun*. 5 (2014) 4666

[Talk#19]

New Strategies Towards Design of Luminescent Metal-Ligand Chromophoric Ensembles, Conjugates and Nano-Assemblies for Sensing and Bioassays

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The major focus of our research is on the molecular design and synthesis of novel inorganic/organometallic metal complexes that may find potential applications as functional metal-based molecular materials. Recent works have shown that novel luminescent metal-based molecular materials could be assembled through the use of various metal-ligand chromophoric building blocks. In this presentation, various design and synthetic strategies together with the successful isolation of new classes of complexes of selected metals will be described. A systematic study of the electronic spectroscopy of the newly synthesized metal complex systems has provided fundamental understanding on the spectroscopic and luminescence origin as well as the structure-property relationship of these complexes. Through a fine control of the interplay amongst various coordination motifs, electrostatic assembly, and non-covalent metallophilic, hydrophobic-hydrophobic and π-π interactions, together with the modulation of various photo-induced electron and energy transfer processes, new strategies towards the rational design of luminescent metal-ligand chromophoric ensembles, conjugates and nano-assemblies that would lead to changes in the absorption and emission characteristics and may find potential applications and functions in luminescence sensing and bioassays, have been made.

[Talk#20]

Organic Nanoparticles for Sensing, Imaging and Therapy

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There is an increasing trend of using organic nanoparticles as active materials for sensing, imaging and therapy applications. We are particularly interested in nanoparticles made from light-harvesting conjugated polymer (CP) and fluorogens with aggregation-induced emission (AIE) characteristics. The recent results show that these nanoparticles could be fabricated to have tunable sizes and emission, with high brightness that is over 10-fold than inorganic quantum dots with a similar dimension. The large absorption cross-sections of CPs have enabled them to be used as photoacoustic contrast agents and for photothermal and photo dynamic therapy.[1] In this talk, I will discuss different strategies to form water-dispersible conjugated polymer nanoparticles and their applications as signal reporters or signal amplifiers for chemical and biological sensing/imaging and therapy. On the other hand, the unique AIE process offers a straightforward solution to the aggregation caused quenching problem faced by traditional fluorophores. In this talk, I will also summarize our recent AIE work to highlight the utility of AIE effect in the development of new fluorescent bioprobes, which allows the use of highly concentrated fluorogens for biosensing and imaging[2] as well as AIE dot-based bioprobes for cancer cell detection, long term cell tracing, and tumor imaging in a noninvasive and high contrast manner.[3]

References

[1] Li, K.; Liu, B. *Polym*. *Chem*. **2010**, 1, 252.
[2] Ding, D.; Li, K.; Tang, B. Z., Liu, B. *Acc. Chem. Res*. **2013**, 2441.
[3] Liang, J.; Tang, B. Z.; Liu, B. *Chem. Soc. Rev*. **2015**, DOI: 10.1039/C4CS00444B.

[Talk#21]

Hetero Triplet Fusion in Acene-Based Organic Light-Emitting Diodes

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The recovery of one emissive singlet state from two non-emissive triplet states through triplet fusion could more than double the theoretical maximum fluorescence efficiency of organic light-emitting diodes (OLEDs), from 5 % to 12.5 %. In practice this is limited to less than 8 %, since random spin statistics dictate that the most likely fusion product is another non-emissive triplet [1]. Directing the fusion process requires additional control, for instance by allowing fusion to occur between dissimilar molecules: hetero-triplet-fusion (HTF). We demonstrate efficient HTF in blends of the blue light-emitting polymer poly(9,9-di-*n*-octylfluorene) (PFO) doped with the soluble Tetracene derivative bis(triisopropylsilylethynyl)tetracene (TTc). Tetracene is a well-known singlet fission material in dense films [2], but when dispersed within a polymer matrix the fission rate is reduced and the singlet state becomes highly emissive. We fabricated OLEDs based on TTc in a standard host-guest structure with PFO and found that the fusion process occurs between triplets across the two distinct molecules. This serves to show that the higher energy, non-radiative triplet states can be avoided in the fusion process by achieving $T_1^A+T_1^B<T_2^{(A\text{ or }B)}$ without the need for complicated synthesis. The flexibility offered by tuning the triplet energies of both host and guest material promise far greater control of the fusion process, and paves the way for future enhancements in device efficiency.

$$T_{1_{PFO}} + T_{1_{PFO}} \xrightarrow{k_{TF_{PFO}}} S_{1_{PFO}} + S_0$$

$$T_{1_{PFO}} + T_{1_{TTc}} \underset{k_{HSF}}{\overset{k_{HTF}}{\rightleftharpoons}} S_{1_{PFO}} + S_0 \text{ or } S_{1_{TTC}} + S_0$$

$$T_{1_{TTc}} + T_{1_{TTc}} \underset{k_{SF_{TTc}}}{\overset{k_{TF_{TTc}}}{\rightleftharpoons}} S_{1_{TTc}} + S_0$$

Figure 1: A schematic of how the singlet fission (SF), triplet fusion (TF), hetero-triplet-fusion (HTF) and potentially hetero-singlet-fission (HSF) rates contribute to the emission from the device and film.

References

[1] C.-J. Chiang, A. Kimyonok, M. K. Etherington, G. C. Griffiths, V. Jankus, F. Turksoy, and A. P. Monkman, Adv. Funct. Mater. **23**, 739 (2013).

[2] M. W. B. Wilson, A. Rao, K. Johnson, S. Gélinas, R. di Pietro, J. Clark, and R. H. Friend, J. Am. Chem. Soc. **135**, 16680 (2013).

[Talk#22]

The Effect of Exciplex Formation on the Performance of Organic Light Emitting Diodes

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There is a considerable controversy about the importance of exciplex formation for efficient Organic light emitting diodes (OLEDs). Exciplex formation can be assigned to localised (loc) or charge transfer (CT) bimolecular excited states. The dominant exciplex excited state configuration depends on two parameters. The relative energy of the HOMO and LUMO levels of the donor and acceptor molecules and the effect of intermolecular conformation (molecular packing) at the interface. Here we analyse three different exciplex configurations using single and double layer devices. The effect of the electric field on the exciplex excited state is analysed and the formation of exciplex, electroplex and electromer is investigated in devices. In solution processable exciplex type devices we have shown that thermal annealing enhances the exciplex formation due to better molecular packing of the donor-acceptor molecules. The time evolution of the exciplex and electroplex population as a function of the electric field and time has been monitored. Slow molecular rearrangements are induced by the electric field at the interface and this is different for different donor-acceptor systems. By proper selection of the donor-acceptor pair and exciplex configuration, optimum energy and charge transfer can be obtained.

[Talk#23]

Photophysical Versus Structural Properties in Hybrid Lead-Halide Perovskites

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Hybrid perovskites represent a new, disruptive, technology in the field of optoelectronics. They have the potential to overcome the performance limits of current technologies and achieving low cost and high integrability. Hybrid halide perovskite, e.g. $CH_3NH_3PbX_3$ [X = Cl, Br, or I], are usually deposited as polycrystalline thin-films with variable mesoscale morphology depending on the growth conditions. The obtained grain size ranges from tens to thousands of nm. Over the last two years the impressive improvement of photovoltaic performance has been driven by radical empirical evolution of the device architecture and processing methodologies. However, there is a considerable lack of understanding of material properties, both as pristine films and their embodiment in a device.

Here we demonstrate that the electron-hole interaction is sensitive to the microstructure of the material. We find that by control of the material processing during fabrication both free carrier and Wannier excitonic regimes are accessible, with strong implications for optoelectronic devices. The long-range order of the organic cation dipole field is disrupted by polycrystalline disorder introducing domain walls where dipole twinning breaks down. The variations in electrostatic potential found for smaller crystallites suppress exciton formation, while larger crystals of the same composition demonstrate an unambiguous excitonic state[1,2]. In addition, we find that it is also possible to design the emissive properties for a single material composition by designing the processing routs[3]. By simply tuning the average crystallite dimension in the film from tens of nanometers to a few micrometers, it is possible to tune the optical band gap of the material along with its photoluminescence lifetime. We show that larger crystallites present smaller bandgap and longer lifetime which correlates to a smaller radiative bimolecular recombination coefficient. We also show that they present a higher optical gain, becoming preferred candidates for the realization of lasing devices.

References

[1] G. Grancini et al, The Journal of Physical Chemistry Letters, 5, 3836, 2014
[2] G. Grancini et al, Exciton Stabilization in Hybrid Lead-Halide Perovskites, manuscript submitted.
[3] V. D’Innocenzo et al, Tuning the light emission properties by band gap engineering in hybrid lead-halide perovskite Journal of the American Chemical Society, 136, 17730, 2014

[Talk#24]

Interfacial Exciton Dissociation at Metal/Organic Interface in Organic Solar Cells

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An investigation of the absorption enhancement and stability of organic solar cells (OSCs) with regular and reverse configurations has been performed. Light absorption in the regular and reverse geometry OSCs was calculated using finite-difference time-domain simulations over the wavelength range from 400 nm to 800 nm. The simulation reveals that OSCs with reverse geometry possess a higher absorption compared to the structurally identical regular configuration OSCs fabricated using an ITO/PEDOT:PSS anode. The reverse configuration OSCs, have an organic functional stack sandwiched between an Al-modified ITO transparent cathode and an opaque bi-layer MoO_3/Ag anode is more efficient than a control regular OSC. The dissociation of excitons at the Al/organic cathode interface in regular geometry OSCs hampers the electron collection. During the deposition of Al contact on the stack of functional organic layers, the energetic metal atoms can induce interfacial defects in the underlying functional organic layers, resulting in forming an adverse charge collection behavior at the complex organic/Al interface. The origin of unfavorable electron collection is mainly due to the compensation of drifted photo-generated electrons at the organic/cathode (Al) interface, which can be eliminated, e.g., by inserting a thin ZnO interlayer between the organic layer and Al electrode. This work clearly reveals that the removal of the unfavorable interfacial exciton dissociation is a perquisite for a significant enhancement in power conversion efficiency in OSCs.

[Talk#25]

Small-Molecule Cathode Interfacial Material Based on Phenanthroline Derivative for High-Performance Organic Photovoltaics

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Cathode interfacial material (CIM) plays an indispensable role for improving the power conversion efficiency and long-term stability of an organic photovoltaic device. Recent years have witnessed an increasingly large number of CIMs, ranging from inorganics to organic small molecules and polymers. We report hereby our recent effort on pursuing organic small-molecule CIM with emphases particularly on concise synthesis/purification and morphology stability. In addition, the CIM that is endowed with good electron transport provides additional advantage for large-area device processing. Besides vacuum deposition, utilizing the newly developed CIM based on solution-processing in inverted organic photovoltaic devices shall be briefly discussed. In situ UPS and XPS experiments were carried out to explain the function of the CIM in the resulting OPV devices.

References

[1] Tan W.-Y., Wang R., Li M., Liu G., Chen P., Li X.-C., Lu S.-M., Zhu H. L., Peng Q.-M., Zhu X.-H., Chen W., Choy W. C. H., Li F., Peng J.B. and Y. Cao, “Lending Triarylphosphine Oxide to Phenanthroline: a Facile Approach to High-Performance Organic Small-Molecule Cathode Interfacial Material for Organic Photovoltaics Utilizing Air-Stable Cathodes”, *Adv. Funct. Mater.* 24, 41(2014),6540-6547.

[Talk#26]

Probing the Ultrafast Vibronic Dynamics of Charge Transfer in Organic Photovoltaic Blends

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Photoinduced charge transfer processes are key to the operation of optoelectronic devices, especially of organic photovoltaics (OPVs). Recently, evidence has come to light that electronic and vibrational coherence may play a role in efficient charge separation in donor acceptor systems, which are used in OPVs [1,2].

Here, we use an ultrafast three-pulse experiment to probe vibrational coherence during the photoinduced charge transfer process in a series of model polymer-fullerene systems. We directly measure the vibrational signatures of the excited states of the system, the singlet exciton and the hole polaron, and find that there is a transfer of vibrational coherence, for certain but not all vibrational modes, between the initially generated singlet exciton and the hole polaron. Furthermore, we find that the vibrational dynamics of the hole polaron formed via charge transfer significantly differ depending on the nature of the fullerene to which the electron is transferred. This allows us to measure the delocalization of the hole polaron wave function.

Our results elucidate the importance of understanding the ultrafast vibrational dynamics related to charge transfer process and how these vibrational modes couple the electronic states allowing for efficient charge generation in organic semiconductors.

References

[1] Y. Song et al., ‘Vibrational coherence probes the mechanism of ultrafast electron transfer in polymer–fullerene blends’. *Nature Commun.* 5:4933, doi: 10.1038/ncomms5933, (2014).

[2] S. Gélinas et al., ‘Ultrafast Long-Range Charge Separation in Organic Semiconductor Photovoltaic Diodes’. *Science* 343, 512-516, (2014).

[Talk#27]

From Engineering Interfaces in Soft Electronic Materials to Efficient Perovskite Photovoltaics

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Present day electronic devices are enabled by design and implementation of precise interfaces that control the flow of charge carriers. However, unlike the well-controlled interfaces in conventional electronics based on silicon and other inorganic materials, organic semiconductor interfaces are relatively poorly characterized and understood. In the first part of the talk I will describe how precise manipulation and control of organic-organic interfaces in a photovoltaic device can increase its power conversion efficiency by 2-5 times in a model bilayer system. Applications of these design principles to practical architectures like bulk heterojunction devices lead to an enhancement in power conversion efficiency from 4.0% to 7.0%. These interface manipulation strategies are universally applicable to any donor-acceptor interface, making them both fundamentally interesting and technologically important for achieving high efficiency organic electronic devices. In the second part of the talk, I will describe a novel solution-processed technique to grow high quality large-area mm-scale perovskite crystals leading to highly efficient (18%) and reproducible solar cells with reduced defect induced recombination. We anticipate that this technique will lead the field towards synthesis of wafer-scale crystalline perovskites necessary for the fabrication of high-efficiency planar solar-cells and be applicable several other material systems plagued by polydispersity, defects and grain boundary recombination in solution-processed thin-films.

[Talk#28]

Magnetic Field Effect in Organic Semiconductor Devices

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Magnetic field effects (MFEs) on the electroluminescence, conductance, and photocurrent of the nonmagnetic organic semiconductor based devices at room temperature have been widely studied. Here, I will first report our investigation of MFEs exerted on photocurrents in N,N'-bis(1-naphthyl)-diphenyl-1,1'-biphenyl-4,4'-diamine (NPB) based devices at room temperature. By varying the layer thickness, applied bias, and interface condition, we achieved interface-exciton/polaron pair-dissociation-dominant and bulk-polaron-detrapping-dominant photocurrent responses. When applying a magnetic field, in addition to the widely documented low MFE (~ 6.5 mT) and high MFE (~ 80 mT), we clearly observed an intermediate MFE (~ 28 mT) that was not reported. The low MFE results from the magnetic field induced decrease of spin-mixing between singlet and triplet polaron pairs. We attribute the high/intermediate MFE to a magnetic field induced rate decrease in triplet-exciton-free-polaron-quenching (T_X-P_{free}) / triplet-exciton-trapped–polaron-detrapping (T_X-P_{trap}), respectively. Then, I will focus on the MFEs on photoluminescence (PL) and the energy transfer processes in NPB, tris- (8-hydroxy-quinolate) aluminium (Alq_3), and 4-(dicyanomethylene)-2-t-butyl-6- (1,1,7,7-tetramethyljulolidyl-9-enyl)-4H-pyran (DCJTB) based fluorescence doped devices. We have found that the magnetic field has no effect on the direct photon absorption and emission process of organic molecules but it affects the energy transfer process from NPB and Alq_3 to DCJTB. The magnetic field induced change of PL intensity for DCJTB emission is found to be much more prominent in Doped NPB device than that in Doped Alq_3 device. The similar results are obtained in time-resolved PL studies. We believe that the Dexter energy transfer via the triplet exciton – polaron interaction is responsible for the observed magnetic field effect on DCJTB PL. In this case, a triplet exciton on donor molecules transfers its energy to form a singlet on the DCJTB molecules by interacting with one polaron in order to conserve the spin. The magnetic field applied reduces this triplet exciton-involved energy transfer rate which leads the decrease of the PL intensity observed.

[Talk#29]

High Field Magneto-luminescence in Organic Semiconductors

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We report the effect of high magnetic field (up to B~6 T) on the light emission from either photo-excited organic semiconductor films or electrically driven organic devices in a wide temperature range. The magneto-photoluminescence (MPL) response consists of a relatively narrow feature in the vicinity of B~0-0.1 T and a broad non-saturating feature up to the highest field employed. Since the emission arises due to singlet exciton (SE, spin S=0) recombination, the magnetic field cannot directly affect the intensity of the radiation. Indirect mechanisms that involve triplet excitons (TE, S=1) or pairs of polarons (PP, pair of S=½ spins) should be considered. TE may affect MPL via spin dependent singlet-triplet intersystem crossing (ISC) which is field dependent since the spin character of each of the TE levels is field dependent [1]. Another TE mechanism involves triplet-triplet annihilation, in which two TEs (generated by ISC) fuse together to produce delayed fluorescence. Naturally, the TE mechanisms should give rise to MPL response that is saturated at fields beyond the zero field splitting (ZFS) parameters of the TE. The ZFS parameters in polymers such as poly(3-hexyl-thiophene) [P3HT] are typically less than 0.1 T, thus TE cannot account for magnetic field effects at fields as high as ~6 T. Also, SE may temporarily charge separate partially to singlet PP or charge transfer excitons (CTE) that spin-mix with the triplet-PP (or CTE) states and eventually fuse back to SE emitting magnetic field dependent delayed fluorescence. Within the PP or CTE species the high field response has been shown to arise from the Δg mechanism at around room temperature [2] or from thermal spin polarization at low temperatures. At high magnetic fields as the temperature decreases thermal spin polarization has an increasing contribution to the MPL. We will discuss these various mechanisms.

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References

[1] B. R. Gautam, T. D. Nguyen, E. Ehrenfreund, and Z. V. Vardeny, “Magnetic field effect on excited-state spectroscopies of π-conjugated polymer films”, Phys. Rev. B, Vol. 85, (2012), 205207.

[2] A. Devir-Wolfman , B. Khachatryan1, B. R. Gautam, L. Tzabary, A. Keren, N. Tessler, Z. V. Vardeny and E. Ehrenfreund, “Short-lived charge-transfer excitons in organic photovoltaic cells studied by high-field magneto-photocurrent”, *Nature Comm.*, Vol. 5, (2014), 4529.

[Talk#30]

Spontaneous Spin Polarization in Charged and Excited Organic Molecules

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Spin polarizations of charged carriers and neutral excitons play important roles in realizing organic spintronic devices. In this work we studied the spin polarization phenomenon of injected charges and excited states in nonmagnetic organic oligomers and copolymers by using both density functional theory calculation and extended Su-Schrieffer-Heeger model including electron-electron interaction as well as spin-orbit coupling effect. Our simulation shows that a charged carrier is spontaneous spin polarized, which has a lower energy than the non-polarized one. This polarization is related with the amount of injected charges and the polymerization of the molecule. By detailed investigation we conclude that the strong electron-lattice interaction in organic materials is responsible for charge induced spin polarization. We indicated that spin polarization behavior in pure organic oligomers is different from that in molecules hybridized with metals. The theoretical picture was confirmed by some recent experimental investigation on excited ferromagnetism in organic compounds.

References

[1] Tarafder K, Sanyal B and Oppeneer P.M, “Charge-induced spin polarization in non-magnetic organic moleculae Alq$_3$”, *Phys. Rev. B*82(2010), 060413-060416.

[2] Dong Hou, Junjie Qiu, Shijie Xie and Avadh Saxena, “Charge-induced spin polarization in thiophene oligomers”, *New J. Physics*. 15(2013), 073044-073054.

[3] Shixuan Han, Hong Jiang, Xiaoxue Li and Shijie Xie, “Spontaneous spin polarization in organic thiophene oligomers”, *Organic Electronics*. 15(2014), 240-244.

[Talk#31]

Photothermoelectric Effect of Organic Semiconductors in Enabling NIR Detection

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Thermoelectric materials are of great interest for promising applications in power generation and refrigeration. Organic semiconductors are recently considered as attractive thermoelectric candidates owing to their intrinsically low thermal conductivity and potential-low cost associated with their ease of low-temperature processing.[1,2] Benefiting from photo-heat-electric conversion in a typical photothermoelectric(PTE) effect, organic PTE material not only allows direct electricity generation but also enables an effective modulation of their thermoelectric properties.

We demonstrated a study of utilizing organic field-effect transistor (OFETs) to achieve effective modulation of thermoelectric properties based on a series of p- and n-type organic semiconductors.[3] Owing to the fine-tuning of carrier concentration and charging level over a wide range by varying the applied gate voltage, the extracted thermoelectric performances from OFETs are consisted with the results of chemically doped films. In particular, it allows investigation PTE properties of organic semiconductors in a FET structure. Several organic semiconductors exhibited light irradiation-intensity and wave-length dependent thermoelectric performances, which are related to the electron-phonon coupling of photo excitation-generated excited states. Moreover, we reported on poly[Cu_x(Cu-ett)]:PVDF, an excellent polymeric thermoelectric composite, possesses unprecedented PTE properties.[4,5] The NIR light irradiation on the poly[Cu_x(Cu-ett)]:PVDF film could induce obvious enhancement in Seebeck coefficient from 52±1.5 to 79±5.0 μV/K. By taking advantage of prominent photo-thermoelectric effect of poly[Cu_x(Cu-ett)]:PVDF, an unprecedented thermoelectric voltage of 12 mV was obtained. This excellent performance enables its promising applications in electricity generation from solar energy and NIR detection to a wide range of light intensities ranging from 1.7 mW/cm^2 to 17 W/cm^2.

References

[1] Zhang Q., Sun Y. M., Xu W. and Zhu D. B., Organic thermoelectric materials: Emerging green energy materials converting heat to electricity directly and efficiently. *Adv. Mater.*, Vol. 26, (2014) pp 6829-6851.

[2] Sun Y. M., Sheng P., Di C. A., Jiao F., Xu W., Qiu D. and Zhu D. B., Organic thermoelectric materials and devices based on p- and n-type poly(metal 1,1,2,2-ethenetetrathiolate)s, *Adv. Mater.*, Vol. 24, (2012), pp 932-937.

[3] Zhang F. J., Zang Y. P., Huang D. Z., Di C. A., Gao X. K., Sirringhaus H. and Zhu D. B., Modulated thermoelectric properties of organic semiconductors using field –effect transistors, *Adv. Funct. Mater.*, In Press.

[4] Jiao F., Zhang F. J., Zang Y. P., Zou Y., Di C. A., Xu W. and Zhu D. B., An easily accessible carbon material derived from carbonization of polyacrylonitrile ultrathin films: Ambipolar transport properties and application in a CMOS-like inverter, *Chem. Commun.*, Vol. 50, (2014), pp 2374-2376.

[5] Huang D. Z., Zou Y., Jiao F., Zhang F. J., Zang Y. P., Di C. A., Xu W. and Zhu D. B., Interface-located photothermoelectric effect of organic thermoelectric materials in enabling NIR detection, *ACS Appl. Mater. Interfaces*, In Revision.

[Talk#32]

Molecular Dynamics Simulations of the Conformational Effects on Optoelectronic Phenomena in Conjugated Semiconducting Oligomers

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There exists a strong interplay between optical response and molecular conformation in organic semiconducting molecules. Particularly, the value of a given dihedral angle between two monomers in a conjugated system often significantly alters its band gap. In addition, the conformational properties of alkyl side-chains on conjugated molecules play an important role in formation of conformational phases, such as the widely-studied ß-phase of poly-fluorene, as well as inhibiting FRET processes between conjugated segments in films.

Given the varied nature of conformation of such molecules, attention has turned recently towards utilising Molecular Dynamics (MD) simulations in order to study such properties. MD simulations allow one to probe the effects of various solvents, lengths of molecule and varieties of side-chain on conformational properties at a relatively low computational cost provided that the appropriate force field parameters are known. However, while there exist reports demonstrating the feasibility and use of such a protocol, there is a lack of consensus on how to generate the appropriate modifications to force field terms in pre-existing force field parameters in order to account for the subtle differences observed due to the presence of a conjugated backbone.

We describe a general protocol to obtain suitable parameters based on modifications to the pre-existing OPLS force field. In particular, we ascertain the required level of DFT theory such that accurate inter-monomer dihedral potentials are obtained. In addition to this, we investigate a number of slight variations to the base molecule, such as varying alkyl side-chain length and increasing the number of monomers, and how they affect the parameterisation procedure. The resulting parameters form a basis for reliably producing MD geometries for use in investigating optical response properties, such as one photon absorption and fluorescence anisotropy decay.

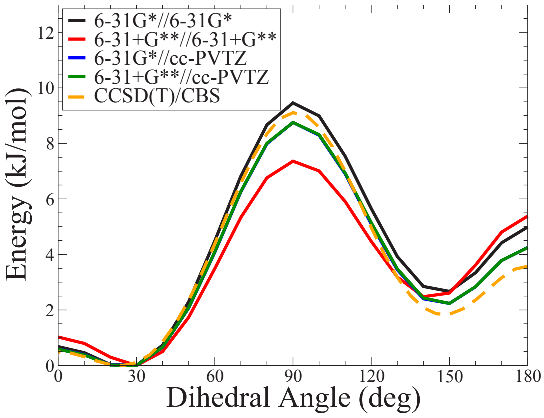

Figure 1: The dihedral energy profile calculated using CAM-B3LYP for a dimer of thiophene with comparison to the CCSD(T)/CBS limit result given in [1]. The basis set X for geometry optimisation and Y for subsequent single-point energy calculation is displayed in the legend as X//Y.

References:

[1] Bloom J. W. G. and Wheeler S. E., “Benchmark Torsional Potentials of Building Blocks for Conjugated Materials”, *J. Chem. Theory Comput.*, Vol. 10, No. 9, (2014), pp. 3647-3655

[Talk#33]

Controlling Cell Functions by Light

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The capability to selectively affect vital functions in cell networks and sub-cell compartments in vitro or in vivo is a mission critical tool in neuroscience and medicine. Optical excitation is one of the main strategies used to achieve high spatial and temporal resolution. Here I will describe recent results and future approaches of cell photostimulation mediated by organic semiconducting polymers. I will show that a range of different cells do respond to photoexcitation through a mediating mechanism of stimulation not yet identified. We studied HEK293 line cell, astrocytes and neurons. Both membrane potential depolarization and hyperpolarization can be obtained, leading to firing and silencing in excitable cells. This opens up a new area of application in bio organic photonics. Among others, the artificial retina implant is a possible application of such interfaces. The status of our research in this direction will be reviewed.

[Talk#34]

Developing Advanced Structural Probes to Identify the Dominant Optical Transitions in Donor-Acceptor Copolymers and Their Impact on Photostability

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Organic semiconductors such as small molecules and conjugated polymers have been demonstrated as the active material in displays, lighting, transistors and solar cells. While innovation in new organic semiconductor materials and solution-processing techniques continues to improve the performance of organic devices, further research is required to gain crucial insights into the fundamental relationships between structure and optoelectronic properties and hence to inform future design strategies. In this talk, I will discuss the key advances on our understanding in developing advanced structural optical probes, in particular resonant Raman spectroscopy, to monitor the properties of these designed molecular architectures [1-10]. As an example, I will introduce our current work based on donor-acceptor copolymers which are an important class of conjugated polymer on account of their chemically tunable energy levels and ambipolar charge transport properties. These materials typically exhibit two strong absorption bands in the UV-visible range, whose natures have previously been explored using theoretical analyses. Here, we experimentally elucidate the electronic origins of these transitions using in-situ resonant Raman spectroscopy. In particular, we identify two dominant electronic transitions for a material comprising diketopyrrolopyrrole (DPP) acceptor and selenophene donor units. The polymer is found to have a wavelength dependent photogradation; good photostability under prolonged excitation in the low energy absorption band, but is much less stable to higher energy excitation. These changes are correlated with the results of ultrafast transient absorption spectroscopy. Our findings provide insight into the design of photostable low energy gap conjugated copolymers for application in organic photovoltaic devices and demonstrate a specific vulnerability of the particular unit. Furthermore, the methods developed here have widespread relevance for the vast range of conjugated molecules whose optoelectronic properties and photostability are critical for fundamental studies and device applications.

References

[1] Tsoi et al., J. Am. Chem. Soc., 133, (2011), 9834-9843.
[2] James et al., ACS Nano 5 (12), (2011), 9824-9835.
[3] Tsoi et al., ACS Nano, 6(11), (2012), 9646-9656.
[4] Wood et al., J. Chem. Phys. 139(6) (2013) 064901
[5] James et al., ACS Nano 7(9) (2013) 7983-7991
[6] Z. Li et al, Nature Comm., 4 (2013) 2227, DOI: 10.1038/ncomms3227
[7] Hollis et al, J. Mater. Chem. A (2014), DOI: 10.1039/c4ta05641h
[8] Kim et al, Adv. Energy Mater. (2014), 1400527
[9] B. R. Lee et al, Nature Comm. 5, (2014) 4840, DOI: 10.1038/ncomms5840
[10]Wade et al, J. Mater. Chem. C (2014), DOI: 10.1039/c4tc01353k

[Talk#35]

Optical Vibrational Control of Charge Transport in Organic Semiconductors

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The ‘soft’ character of organic materials leads to strong coupling between molecular nuclear and electronic dynamics.[1] This coupling opens the way to control charge transport in organic molecules[2] and electronic devices by exciting molecular vibrational motions. However, despite encouraging theoretical predictions, experimental realization of device control has remained elusive. Here we demonstrate experimentally that photoconductivity in a model organic optoelectronic device can be controlled by the selective excitation of molecular vibrations.

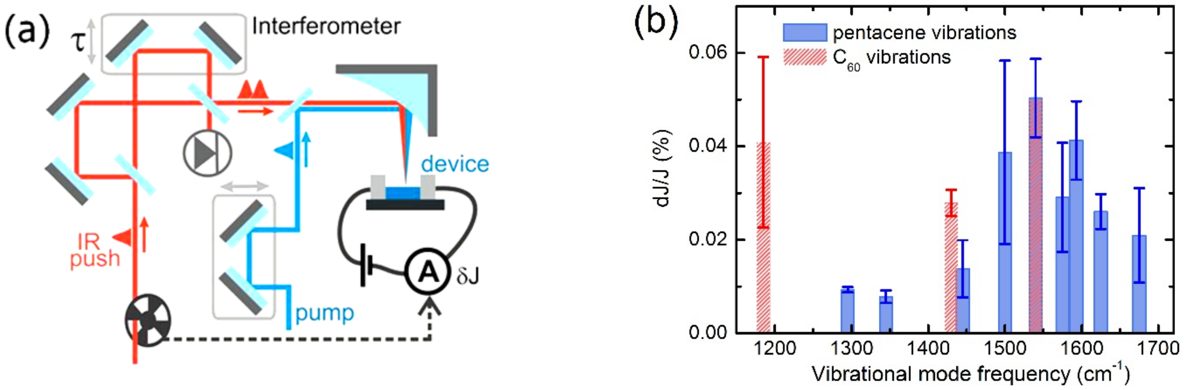

Figure 1. *(a) The layout of the time- and frequency-resolved PPP experiment. (b) The influence of different vibrations on device photocurrent, estimated by normalizing the amplitude of the PPP signal to the absorbed IR intensity.*

Using an ultrafast infrared laser system (fig.1a) to create a coherent superposition of vibrational motions in a pentacene/C_{60} photoresistor, we observe that excitation of certain modes in the 1500-1700 cm^{-1} region leads to photocurrent enhancement.[3] Excited vibrations affect predominantly trapped carriers. The effect depends on the nature of the vibration and its mode-specific character (fig.1b) can be well described by the vibrational modulation of intermolecular electronic couplings. ‘Vibrational control’ thus presents a new tool for studying electron-phonon coupling and charge dynamics in (bio)molecular materials.

References

[1] Galperin, M., Ratner, M.A., Nitzan, A. & Troisi, A. “Nuclear Coupling and Polarization in Molecular Transport Junctions: Beyond Tunneling to Function”, *Science* 319, (2008) 1056.
[2] Delor M., Scattergood P.A., Sazanovich I.V., Parker A.W., Greetham G.M., Meijer A.J.H.M., Towrie M., Weinstein J.A., “Toward control of electron transfer in donor-acceptor molecules by bond-specific infrared excitation”, *Science* 346, (2014) 1492.
[3] Bakulin A.A., et al. “Mode-selective vibrational control of charge transport in pi-conjugated molecular materials”, *arXiv preprint arXiv:1503.00777* (2015)

[Talk#36]

Spontaneous Fluctuation of Transition Dipoles Revealed by Single-molecule Spectroscopy

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The efficiency of an organic light-emitting diode (OLED) strongly depends on the microscopic orientation of transition dipole moments of the molecular emitters. It would be desirable to control the dipole orientation to maximize the out-coupling efficiency. In conventional measurement techniques, however, it is not possible to determine the polarization anisotropy of the individual emitter due to ensemble averaging in solution or bulk film. In contrast, single-molecule spectroscopy is capable of acquiring microscopic insight into the spatial and temporal arrangement of transition dipole moments from single luminescent particles. Recent measurements showed that the dipole moment orientation, responsible for fluorescence, can fluctuate spontaneously in synthesized planar carbazole macrocycles by using polarization resolved photoluminescence measurements [1].

Similar fluctuations also exist for phosphorescent molecules as used in OLEDs. We investigated the prototypical model triplet emitter tris(1-phenylisoquinoline)iridium(III) (Ir(piq)3) with regards to its emission polarization properties one molecule at a time [2]. Here, spontaneous symmetry breaking occurs in the excited state, leading to a random selection of one of the three ligands to form a charge-transfer state with the metal in the center of the molecule (Fig. 1). This nondeterministic localization is revealed in switching of the linear polarization of phosphorescence. Polarization scrambling is likely to raise out-coupling efficiency and should be taken into account when deriving molecular orientation of the guest emitter within the OLED host from ensemble angular emission profiles.

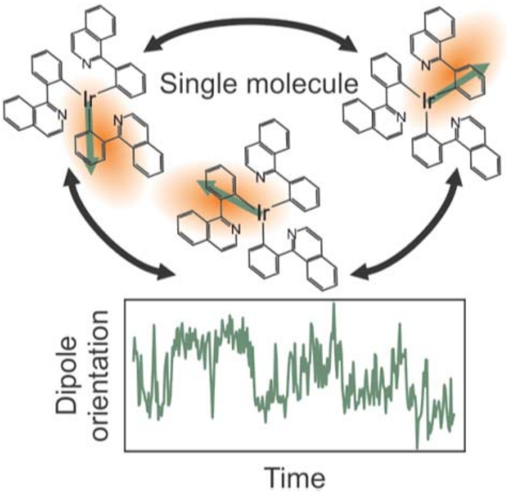

Figure 1.

References

[1] Aggarval V., Thiessen A., Idelson A., Kalle D., Würsch D., Stangl T,. Steiner F., Jester S.-S., Vogelsang J., Höger S., Lupton J.M., “Fluctuating exciton localization in giant Pi-conjugated spoked-wheel macrocycles”, Nature Chem., Vol. 5, (2013), p. 964

[2] Steiner F., Bange S., Vogelsang J., Lupton J.M., “Spontaneous fluctuations of transition dipole moment orientations in OLED triplet emitters”, J. Phys. Chem. Lett, Vol. 6, (2015), p. 999

[Talk#37]

Decoherence and Energy Relaxation within Charge Transport Process in Crystalline Organic Semiconductors

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We investigate the decoherence (DC) and energy relaxation (ER) within the charge transport process in the mixed quantum-classical dynamics (MQCD) model of crystalline organic semiconductors. Both of the DC and ER, which are missing in the classical treatment of MQCD through the ensemble average of the phonon degree of freedom, are believed to play crucial roles for the carrier to keep as a localized object and to move along the direction of an external electric field. (1) Within the dynamical disorder (mixed quantum-classical) model for charge carrier transport, [1] the decoherence process is taken into account via a phenomenological site or state measurement, that makes the carrier to be restricted as a localized object while the transport behaves as band-like one; [2] (2) We complement phenomenologically the energy relaxation in carriers' transport within the mixed quantum-classical electron-phonon interacting model, to meet the Boltzmann distribution for carriers in a process close to equilibrium; [3] (3) We show that both the DC and ER are necessary to achieve the direct current response of external electric field and realize the direct calculation of carrier's mobility. [4] Furthermore we show that the Einstein relation is still applicable under low electric field (~10^4 V/cm). Besides, the mobility predicted in this case is smaller than that from the Ehrenfest dynamics, which might account for the gap of the mobility values from the Ehrenfest dynamics and full quantum-mechanical results using the Kubo formula. [5]

References

[1] Troisi A. and Orlandi G., "Charge-Transport Regime of Crystalline Organic Semiconductors: Diffusion Limited by Thermal Off-Diagonal Electronic Disorder", *Phys. Rev. Lett.,* Vol. 96, No. 8, (2006) pp 086601.

[2] Yao Y., Si W., Hou X. and Wu C.-Q., "Monte Carlo simulation based on dynamic disorder model in organic semiconductors: From coherent to incoherent transport", *J. Chem. Phys.*, Vol. 136, No. 23, (2012), pp 234106.

[3] Si W. and Wu C.-Q., "Near Equilibrium Carriers' Distribution in the Mixed Quantum-Classical Dynamics of Charge Transport for Crystalline Organic Semiconductors", to be published.

[4] Dong J., Si W. and Wu C.-Q., "Decoherence and Energy Relaxation on the Carrier's Transport in Crystalline Organic Semiconductors", to be published.

[5] De Filippis G., Cataudella V., Mishchenko A.S., Nagaosa N., Fierro A., and de Candia A., "Crossover from Super- to Subdiffusive Motion and Memory Effects in Crystalline Organic Semiconductors", *Phys. Rev. Lett.*, Vol. 114, No. 8, (2015), pp 086601.

[Talk#38]

Tracking Charge Photogeneration in 3-phase Polymer:Fullerene Blends

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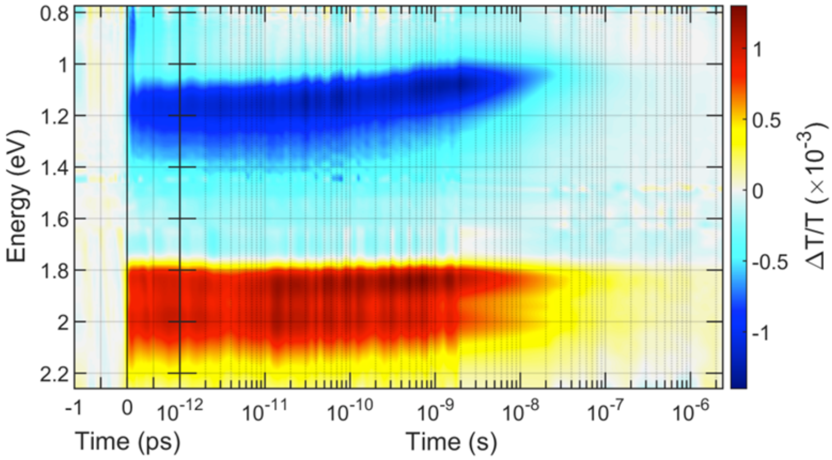
The mechanism by which charge pairs escape their Coulombic attraction to generate photocurrent in organic photovoltaic cells remains elusive. Our recent resolution of exciton delocalization[1] and discovery that long-range charge separation occurs within carrier cooling timescales[2], prompted us to explore the role of blend morphology on this process.

In a series of polymer:fullerene blends, we investigated the correlation of free charge yields with dynamic parameters including prompt vs. delayed charge generation pathways, and the spectral evolution of holes from intermixed to pure polymer regions. In a specific case study, we studied a series of closely related alternating thiophene-benzothiadiazole copolymers in which the tuned curvature of the polymer backbone controls the nature and degree of polymer-fullerene intermixing.[3] Free charge generation is most efficient in the 3-phase morphology that features intimately mixed polymer:PCBM regions amongst neat polymer and PCBM phases. TA spectral dynamics (see figure below) and polarization anisotropy measurements reveal the migration of holes from intermixed to pure polymer regions of such blends, which contrasted with observations in 2-phase blends.

We conclude that the energy gradient between intermixed and phase-pure regions may be sufficient to drive separation of charge pairs initially generated in intermixed regions.



References

[1] Chen, K., Barker, A. J., Reish, M. E., Gordon, K. C. & Hodgkiss, J. M. “Broadband Ultrafast Photoluminescence Spectroscopy Resolves Charge Photogeneration via Delocalized Hot Excitons in Polymer:Fullerene Photovoltaic Blends” *J. Am. Chem. Soc.* 135 (2013) 18502-18512.
[2] Barker, A. J., Chen, K. & Hodgkiss, J. M. “Distance Distributions of Photogenerated Charge Pairs in Organic Photovoltaic Cells” *J. Am. Chem. Soc.* 136 (2014), 12018–12026.
[3] Lee, W., Kim, G.-H., Ko, S., Yum, S., Hwang, S., Cho, S., Shin, Y., Kim, J. Y. & Woo, H. Y. “Semicrystalline D–A Copolymers with Different Chain Curvature for Applications in Polymer Optoelectronic Devices” *Macromolecules* 47 (2014), 1604-1612.

[Talk#39]

Charge-transfer Dynamics and Vibrational Coherence in Polymer/Fullerene Blends

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Charge photogeneration in organic solar cells is facilitated by the dissociation of excitons at a donor/acceptor interface. The ultrafast timescale of charge separation demands sophisticated theoretical models and raises questions about the role of coherence in the electron-transfer mechanism. In this presentation, we will summarize our recent experimental efforts on investigating electron transfer dynamics in polymer/fullerene blends using two-dimensional electronic spectroscopy (2D ES). We investigated[1] ultrafast electron transfer in poly(3-hexylthiophene) (P3HT) /PCBM blends and utilized 2D ES to directly monitor different pathways of electron transfer. This work provides experimental evidence on hot electron transfer and sheds light on the electron transfer mechanism. Specifically, the similar dephasing time of vibrational coherences on both the initially photogenerated exciton and charge-transfer product (more specifically, P3HT cation) indicates that the wavefunction of the P3HT cation exhibits a similar spatial extent as the photogenerated exciton. To further explore the effect of coherences on the electron transfer mechanism, we recently proposed[2] a more robust protocol that utilizes 2D coherence amplitude maps to separate the vibrational coherence from ground- and excited- electronic states. By applying this data-analysis method to P3HT films, we found that the vibrational coherence from excited electronic states had a dephasing time of ~ 244 fs. The long dephasing time of the vibrational coherence suggests that it might be involved in the electron transfer process (< 50 fs) in P3HT/PCBM blends. We are in the process of extending this methodology further to investigate the dynamics of ‘dark’ charge-transfer states in polymer/fullerene blends.

References

[1] Song Y., Clafton S.N., Pensack, R.D., Kee, T.W., and Scholes, G.D., “Vibrational coherence probes the mechanism of ultrafast electron transfer in polymer–fullerene blends”, Nature Communication, Vol. 5, No. 4933, (2014), pp 1-7

[2] Song Y., Hellmann. C., Stingelin, N., and Scholes, G.D., “The separation of vibrational coherence from ground- and excited-electronic states in P3HT film”, *The Journal of Chemical Physics*, Vol. 142, No. 212410, (2015), pp 1-11.

[Talk#40]

Time-dependent Wavepacket Diffusive Method and Its Applications to Carrier Quantum Dynamics in Organic Materials

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The carriers in organic materials commonly follow hopping-type motions because of strong carrier-phonon interactions. However, they can also present a band-like behaviour in well-performed organic crystals or mixed inorganic-organic materials. Therefore, the carrier quantum dynamics should be described by a unified way covering from band-like to hopping-type motions. Such a unified method for large systems still meet a great challenge in theoretical chemistry. Focusing on this problem, we have proposed a time-dependent wavepacket diffusion method (TDWPD)[1,2]. In the method, the effects of carrier-phonon interaction and inter- or intra-molecular electronic couplings are considered as the fluctuations on carrier dynamics. It has been demonstrated that the TDWPD computational cost is similar to that of mixed quantum-classical methods for complex systems, but it overcomes their deficiency that the detailed balance principle is broken down, and it also includes nuclear tunnelling effect and correctly predicts a long time dynamics behaviour. We further present how to combine electronic structure calculations and molecular dynamics simulations[3,4] with the TDWPD to reveal the carrier dynamics in realistic organic semiconductors, such as exciton energy relaxation and dissociation, mobility of electron and hole[5,6].

References

[1] XX Zhong and Y Zhao, J. Chem. Phys., 135, 134110(2011)
[2] XX Zhong and Y. Zhao, J. Chem. Phys., 138, 014111(2013)
[3] Y Zhao and WZ Liang, Chem. Soc. Rev., 41, 1075(2012)
[4] JH Yang, WW Zhang, YB Si, and Y Zhao, J. Phys. Chem. B, 116,14126(2012)
[5] WW Zhang, XX Zhong and Y Zhao, J. Phys. Chem. A, 116, 11075(2012)
[6] L Han, XX Zhong, WZ Liang and Y Zhao, J. Chem. Phys., 140, 214107(2014)

[Talk#41]

RISC from High-lying Triplet to Singlet: Optical Probes and Application for OLEDs

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When a singlet state(S) nonradiatively passes to a triplet state(T), or conversely a T transitions to a S, that process is known as intersystem crossing(ISC, S to T) or RISC(T to S). Because the spin of the excited electron is reversed, the time scale of ISC is relative slow with the order of 10^{-8} to 10^{-3} s, one of the slowest forms of relaxation. As a result, the probability of this process occurring is sufficiently low. In some cases this process can be accelerated when the vibrational levels of both S and T states overlap or the spin/orbital interactions in such molecules are substantial. In heavy-atom molecules with strong spin-orbit coupling, ISC becomes more favourable, and the heavy metal complexes behavior strong phosphorescence for highly efficient OLEDs. In very few cases, RISC from lowest triplet states (T_1) to lowest singlet states (S_1) can become a dominated process, typically as the thermally-activated delayed fluorescence (TADF) and triplet-triplet annihilation (TTA), but it is great challenging to obtain highly exciton utilization efficiency (η_r) and fluorescence efficiency (η_{PL}). In the end 1969, some aromatic compounds were found that the RISC can occur from the high-lying triplet energy levels to the singlet manifold(T_n (n>1) → S_1)[1], but the efficiency of such delayed fluorescence is too low to find a suitable application. Here, we innovatively rejuvenated this “sleeping” photophysical process by utilizing it to break the exciton statistics limit in OLEDs. Arduous efforts are made to developing fluorescent materials with combination of high photoluminescence efficiency and effective RISC through appropriate molecular design in a series of donor-acceptor (D-A) material systems. The experimental and theoretical results indicate that these materials exhibit hybridized local and charge-transfer excited state (HLCT), which achieve a combination of the high radiation from local excited state (LE) and the high $T_m \rightarrow S_n$ ($m \geq 2$, $n \geq 1$) conversion along charge-transfer excited state (CT). As expected, the devices exhibited favorable external quantum efficiency (EQE) and low roll-off, and especially the exciton utilization efficiency exceeding the limit of 25%.[2,3]

References

[1] Keller R.A., “Excited triplet — singlet intersystem crossing”, *Chem. Phys. Lett.*, Vol.3, No.1, (1969), pp 27-29
[2] Yao L., Yang B., Ma Y.G., “Highly Efficient Near-Infrared Organic Light-Emitting Diode Based on a Butterfly-Shaped Donor-Acceptor Chromophore with Strong Solid-State Fluorescence and a Large Proportion of Radiative Excitons”, *Angew. Chem. Int. Ed.*, Vol.53(2014), pp 2119-2123
[3] Yao L., Yang B., Ma Y.G., “Progress in Next-Generation Organic Electroluminescent Materials: Material Design Beyond Exciton Statistics”, *Sci. China. Chem.,* Vol.,57(2014), pp 335-345.

[Talk#42]

Tailored Polymers for Efficient Thermal Activated Delayed Fluorescence. Towards Printable TADF OLEDs

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Thermally assisted delayed fluorescence (TADF), also known as E-type delayed fluorescence, has gained very rapid interest as a mechanism to improve OLED efficiencies. TADF allows harvesting 100% of the excitons formed from charge recombination, without requiring the use of expensive and scarce materials such as iridium or platinum. The observation of efficient TADF requires the 'dark' triplet excited states to be easily converted into emissive singlet states by reverse intersystem crossing, i.e. using the thermal energy to assist reverse intersystem crossing and promote the up-conversion of lower triplet states into more energetic but emissive singlet states. [1]

So far no TADF has been observed in oligomers and conjugated polymers for use in solution-processed PLEDs. The advantages of solution processing fabrication methods, such as very-high-speed deposition over large substrate areas, that spin-coating and spray-on deposition methods and ink-jet printing offer seems therefore unavailable for TADF devices. This represents a limitation to this type of devices, and a serious threat to the use of polymers and oligomers in the OLED industry, which are thus unable to reach the high device efficiencies presented by TADF devices nowadays.

Several reasons are given to explain why the observation of TADF is difficult in oligomers and polymers. Firstly, simultaneously achieving small ΔE_{ST} and suppressing internal conversion is very difficult in molecules containing many atoms, secondly in polymers and also in oligomers, intramolecular triplet-triplet annihilation (TTA) is often operative and efficiently quenching the triplet states. It is mainly to avoid TTA that small TADF molecules are dispersed in hosts with high triplet energy levels. Unfortunately host molecules often influence the photoluminescent (PL) and electroluminescent (EL) properties of TADF emitters, causing large variations on the emission yield and lifetime due to host-guest exciplex formation,[2] and heterogeneity on the host-guest molecular geometries.[3]

Here we report for the first time efficient TADF in solution-processed pristine polymer films, with no need of using high-triplet level host materials to disperse the emitter. This work elucidates the complex and rich photophysics of TADF polymer materials and addresses the impact of molecular structure and energy ordering of electronic states on the application of these materials in PLED devices, giving clear guidelines for the design of new emitters, and opening the way for TADF to be explored in solution-processed PLEDs as a way to increase device efficiencies.

References

[1] F. B. Dias, K. N. Bourdakos, V. Jankus, K. C. Moss, K. T. Kamtekar, V. Bhalla, J. Santos, M. R. Bryce, A. P. Monkman, *Adv. Mater.* **2013**, 25, 3707.
[2] G. Méhes, K. Goushi, W. J. Potscavage, Jr., C. Adachi, *Organic Electronics* **2014**, 15 2027.
[3] V. Jankus, P. Data, D. Graves, C. McGuinness, J. Santos, M. R. Bryce, F. B. Dias, A. P. Monkman, *Adv. Funct. Mater.* **2014**, 24, 6178.

[Talk#43]

Utilizing the Doublet Emission of Neutral π-radical to Break the 25% Upper Limit of Internal Quantum Efficiency of OLEDs

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The triplet harvesting is a main challenge in the field of organic light-emitting devices (OLEDs), due to that the radiative decay of triplet is spin-forbidden. Here, we propose a new kind of OLEDs utilizing the emission from doublet to bypass the transition problem of triplet for the first time [1].

In this kind of OLEDs, organic open-shell molecules, neutral pi radicals, are used as the emitter. For the open-shell molecule, there is only one unpaired electron in the highest singly occupied molecular orbital (SOMO). When this electron is excited into the lowest singly unoccupied molecular orbital (SUMO), the SOMO is empty. Thus, its transition back to the SOMO is always allowed in despite of its spin state.

(4-N-carbazolyl-2,6-dichlorophenyl)bis(2,4,6-trichlorophenyl)methyl (TTM-1Cz), a kind of photoluminescent radical [2], was used as the emitter. We fabricated the OLEDs with the structure of ITO / NPB (30 nm) / TTM-1Cz : CBP (wt. 5 %, 40 nm) / TPBi (35 nm) / LiF (0.8 nm) / Al (100 nm). The maximum external quantum efficiency of the OLED is 2.4 % at 7 V, which lies in the same levels as most deep-red / near-infrared OLEDs. In addition, we note that the long lifetime of the delayed fluorescence ranging from microseconds to milliseconds may prevent the application of TADF emitters in high-end displays due to the long response time of device. Here, we measured the lifetime of the excited states of TTM-1Cz. The lifetime was fitted to be 25.2 ns, which is much shorter than that of the TADF emitters, indicating the potential application in displays. The Magneto-electroluminescence measurement reveals that the spin configuration of excited states of TTM-1Cz is doublet. Our results pave a new promising way to obtain 100 % internal quantum efficiency of OLEDs. We anticipate that our work will be a start-point for further research, leading to high performance organic open-shell-compounds based OLEDs [3].

References

[1] Li F., “A kind of OLEDs based on the transition of doublet electron of neutral pi radicals”, *Chinese patent*, 201410018393.9 (01/2014).

[2] Velasco D., Castellanos S., López M., López-Calahorra F., Brillas E., and Juliá, L., “Red Organic Light-Emitting Radical Adducts of Carbazole and Tris(2,4,6-trichlorotriphenyl)methyl Radical That Exhibit High Thermal Stability and Electrochemical Amphotericity”, *Journal of Organic Chemistry*, 72, 20, (2007), 7523-7532.

[3] Peng Q., Obolda A., Li F., “Organic light-emitting diodes using neutral π-radical as emitter: the emission from doublet” submitted.

[Talk#44]

Exciplex Way From Blue to Red, Novel TADF Emitters

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New emitters that can harvest both singlet and triplet excited states to give 100% internal conversion of charge into light, are required to replace Ir based phosphors in organic light-emitting diodes (OLEDs). Molecules that have a charge transfer excited (CT) state can potentially achieve this through the mechanism of thermally activated delayed fluorescence (TADF). An innovative idea to generate photons in electroluminescent diodes is to use an exciplex of two different low molecular weight compounds, one of which is electron-donating (D) and the other electron-accepting (A) (Figure 1). This optoelectronic system, where the active layer is bimolecular, allows greater freedom in choice of organic compound. The wavelength of the emission in such a system is not dependent on the band-gap value of a single compound, but rather that of the exciplex. This results in the HOMO energy being that of the electron-donating compound and LUMO energy defined by the electron-accepting compound. Exciplexes are characterized by a very small gap between the singlet and triplet state. This feature indicates that the use of this type of excited state will be ideal for use in devices using an E-type delayed fluorescence process.

Here, we show the examples and tools used to tailor the emission of the exciplex from red to blue, and present the compounds and mixtures that form these exciplex states.

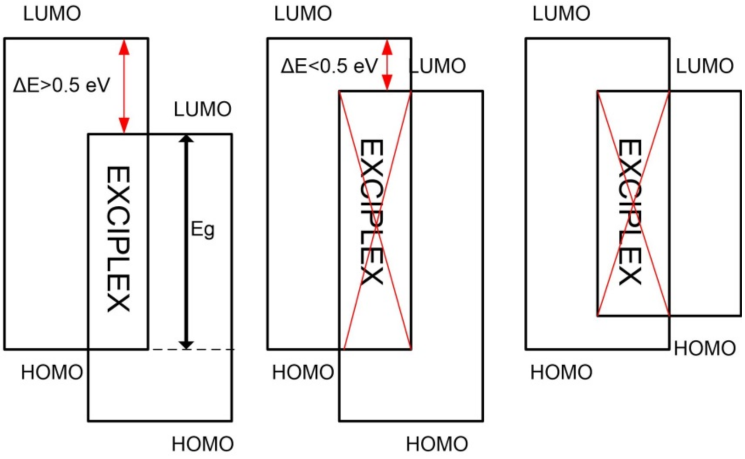

Figure 1 – General scheme of exciplex emitters.

[Talk#45]

Modeling Aggregation Effects on Molecular Light-emitting Quantum Efficiency and Spectroscopy

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The aggregation effects on both the light-emitting quantum efficiency and spectroscopy are investigated by the time-dependent vibration correlation formalism [1] coupled with time-dependent density-functional theory calculations. The exotic aggregation induced emission (AIE) phenomena is explained quantitatively by aggregation reduced non-radiative decay rate due to the restriction on phenyl ring twisting [2]. We propose to probe the AIE mechanism through resonant Raman Spectroscopy [3]. We further discuss the excitonic effect on the non-radiative decay rate for molecular aggregate. We found that the intermolecular electrostatic interaction dominates excitonic coupling for the non-radiative decay, since the latter is governed mostly by intramolecular vibronic couplings [4].

References

[1] Peng Q., Niu Y L, Shi QH, Gao X, Shuai ZG, Correlation Function Formalism for Triplet Excited State Decay: Combined Spin-orbit and Non-adiabatic Couplings, *J. Chem. Theory Comput.* 9(2), 2013, 1132-1143

[2] Shuai ZG, Peng Q, Excited states structure and processes: Understanding organic light-emitting diodes at the molecular level, *Physics Reports* 537(4), 2014, 123-156.

[3] Zhang T, Ma HL, Niu YL, Li WQ, Wang D, Peng Q, Shuai ZG, Liang WZ, Spectroscopic Signature of the Aggregation-Induced Emission Phenomena Caused by Restricted Non-radiative Decay: A Theoretical Proposal. *J. Phys. Chem. C*, 119(9), 2015, 5040-5047.

[4] Zhu LL, Li WQ, Niu YL, Peng Q, Shi Q, Shuai ZG. In preparation.

[Talk#46]

The Optical Properties of Conjugated Materials and their Aggregates: Towards Imaging of Films and Devices

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Applications of semi-conducting conjugated polymers, such as MEH-PPV, in organic lighting and displays drive the need to understand how morphology affects function. One of the most critical morphological aspects of these systems is their stacking interactions or aggregation. Important functional features that are sensitive to aggregation are the emission spectra, quantum yields and the charge-transport properties. Our group uses fluorescence spectroscopy and microscopy to probe variations in the vibronic structure, quantum yields and fluorescence lifetimes between individual aggregates of PPV- and thiophene-based polymers and oligomer model compounds.1-3 From fluorescence lifetime imaging data of individual aggregates, a morphological model has been developed that is supported by more recent measurements of ultra-fast wavelength-dependent exciton-exciton annihilation dynamics via fluorescence upconversion measurements. Together, these methods provide a detailed probe of the structure and packing properties of conjugated materials in the aggregated state and in films. In addition, more recently we have been investigating how the emission properties of these materials are altered when they are deposited on metal surfaces, specifically plasmonic and sub-plasmonic metal films. Surprisingly, MEH-PPV deposited on thin sub-plasmonic metal films is equally as emissive as that deposited on glass. Moreover, the metal film causes a dramatic increase in the photo-stability of the polymer film, even under ambient oxygen. Experiments to understand the mechanism of this unusual effect will be described.

References

[1] Sherwood G. A., Cheng R., Smith T. M., Werner J. H., Shreve A. P., Peteanu L. A., Wildeman J., "Aggregation Effects on the Emission Spectra and Dynamics of Model Oligomers of MEH-PPV", *J. Phys Chem. C*, Vol. 113, (2009), pp.18851-18862.

[2] Peteanu L. A., Sherwood G. A., Werner J. H., Shreve A. P., Smith T. M., Wildeman J., "Visualizing Core-Shell Structure in Substituted PPV Oligomer Aggregates Using Fluorescence Lifetime Imaging Microscopy (FLIM)", *J. Phys. Chem. C*, Vol. 115, (2011), pp.15607-15616.

[3] So W. Y., Hong J., Kim J. J., Sherwood G. A., Chacon-Madrid K., Werner J. H., Shreve A. P., Peteanu L. A., Wildeman J., "Effect of Solvent Properties on the Spectroscopy and Dynamics of Alkoxy-Substituted PPV Oligomer Aggregates", *J. Phys. Chem. B.*, Vol.116, (2012), pp. 10504-10513.

[Talk#47]

Highly Solid-State Emissive Organic Fluorescent Materials

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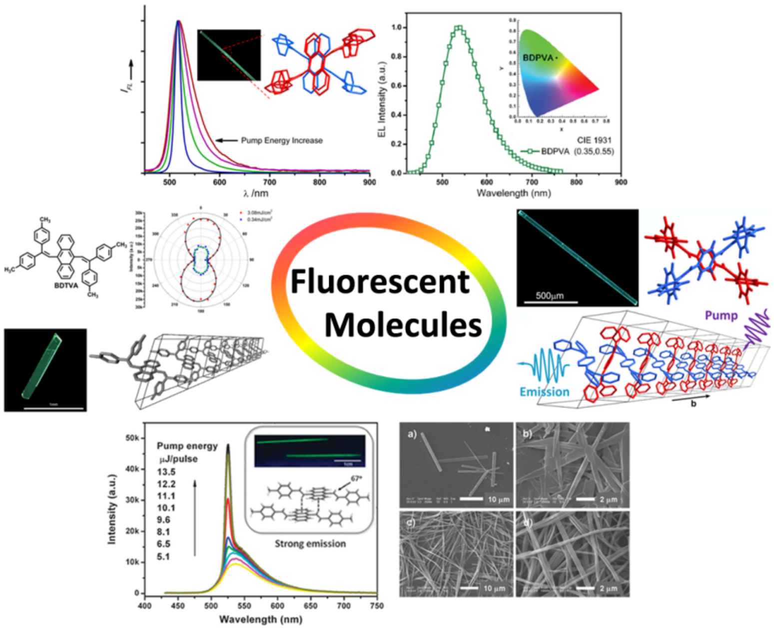
Organic fluorescent materials with high solid state fluorescence efficiency have attracted intense attention for their distinct photoelectric properties and wide potential applications in the field of organic light-emitting diodes, organic field effect transistors, organic solid-state lasers, sensors and memories. Massive effort has been spent on the molecular design and modification, as well as the related applications of organic fluorescent materials which show strong fluorescence in the solid. In our group, a series of organic fluorescent materials with high solid state fluorescence efficiency have been designed and synthesized. The investigation of the related mechanism for the high solid state fluorescence efficiency indicated that the restriction of the torsional motions by the intermolecular interaction leads to the enhanced fluorescence in aggregates. In addition, the steric hindrance arising from the terminal groups makes the center luminophore not too close with others in the aggregates. As a result, there is a large distance and no obvious face-to-face π–π interaction between adjacent molecules, which contributes to the emission in the solid state. The study on the photoelectric properties of these organic fluorescent materials shows the bright future of the materials in the fields of organic solid lasers, electroluminescence and sensors.



References

[1] Zhang J., Xu B., Chen J., Ma S., Dong Y., Wang L., Li B., Ye L., and Tian W., *Adv. Mater.*, Vol. 26, (2014), pp 739-745.

[2] Chen J., Ma S., Zhang J., Li B., Xu B., and Tian W., *ACS Photonics*, Vol. 2, (2015), pp 313-318.

[3] Ma S., Zhang J., Qian J., Chen J., Xu B., and Tian W., *Adv. Optical Mater.* (2015), DOI: 10.1002/adom.201400572.

[4] Xu B., Fang H., Dong Y., Chen F., Chen Q., Sun H., and Tian W., *New J. Chem.*, Vol. 34, (2010), pp 1838-1842.

[5] Dong Y., Xu B., Zhang J., Lu H., Wen S., Chen F., He J., Li B., Ye L., and Tian W., *CrystEngComm*, Vol. 14, (2012), pp 6593-6598.

[Talk#48]

Putting Organic and Organic/Inorganic Hybrid Materials to Work for Efficient Solar Energy Conversion

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Organic and organic/inorganic hybrid materials with novel optoelectronic functionalities play a key role in developing the new generation of solar cells. In particular, the performance of sensitized solar cells and solar fuel generation devices largely determined by these materials in conjunction with suitably designed nanostructures for light harvesting, charge separation, transport and catalysis. This presentation will highlight some of our recent results in understanding, interfacing and assembling these materials for efficient solar energy conversion. First, I will focus on the development of new metal-free organic sensitizers, organic/inorganic light absorbers, and mesoscopic structures interfaces for both sensitized and thin film solar cells as well as solar fuel devices. In particular, power conversion efficiency (PCE) of our solar cell devices over 15% can now be readily obtained with good stability and at low-cost by judiciously engineering the multiple material properties and synergies.

References

[1] "Hybrid Halide Perovskite Solar Cell Precursors: The Colloidal Chemistry and Coordination Engineering behind Device Processing for High Efficiency Dots". Keyou Yan, Mingzhu Long, Tiankai Zhang, Zhanhua Wei, Haining Chen, Shihe Yang, Jianbin Xu, *J. Am. Chem. Soc.*, **137**, 4460-4468 (2015).

[2] "High-performing Hole Extraction Layer for Inverted Planar Perovskite Solar Cells from Sol-gel Processed NiO Nanocrystals". Zonglong Zhu, Yang Bai, Teng Zhang, Zhike Liu, Xia Long, Zhanhua Wei, Zilong Wang, Lixi Zhang, Jiannong Wang, Feng Yan, Shihe Yang, *Angew. Chem., Int. Ed.*, **53**, 12571-12575 (2014).

[3] "Stronly Coupled Graphene and FeNi Double Hydroxide Hybrid as an Excellent Electrocatalyst for Oxygen Evolution Reaction". Xia Long, Jinkai Li, Shuang Xiao, Keyou Yan, Zilong Wang, Haining Chen, Shihe Yang, *Angew. Chem., Int. Ed.*, **53**, 7584-7588 (2014).

[4] "Efficiency Enhancement of Perovskite Solar Cells through Fast Electron Extraction: the Role of Graphene Quantum Dots". Zonglong Zhu, Jiani Ma, Zilong Wang, Cheng Mu, Zetan Fan, Lili Du, Yang Bai, Louzhen Fan, He Yan, David Lee Phillips, Shihe Yang, *J. Am. Chem. Soc.*, **136(10)**, 3760-3763 (2014).

[5] "A Quasi-Quantum Well Sensitized Solar Cell with Accelerated Charge Separation and Collection", K. Yan, Lixia Zhang, Jianhang Qiu, Yongcai Qiu, Zonglong Zhu, Jiannong Wang, Shihe Yang, *J. Am. Chem. Soc.* **135**, 9531 (2013).

[6] New Dithiafulvenyl Donor for High-Eff. DSSCs: Synthesis and Demonstration of a Family of Metal-Free Organic Sensitizers", K. Guo, K. Yan, X. Lu, Y. Qiu, Z. Liu, J. Sun, F. Yan, W. Guo, S. Yang, *Org. Lett.* **14**, 2214 (2012).

[7] "Double-layered Photoanodes from Variable-Size Anatase TiO_2 Nanospindles: A Promising Candidate for High-Efficiency Dye-Sensitized Solar Cells", Yongcai Qiu, Wei Chen, Shihe Yang, *Angew. Chem., Int. Ed.* **49**, 3675 (2010).

[Talk#49]

Modulating Electron - Hole Interaction in a Hybrid Lead Halide Perovskite with Electric Field

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Despite rapid developments in both photovoltaic and light emitting device performance, the understanding of the optoelectronic properties of hybrid lead halide perovskites is still poor. In particular, the polarizability of the material[1,2], the presence of molecular dipoles, and their influence on the dynamics of the photo-excitations[3] has remained an open issue to be clarified. Here, we investigate the effect of an applied electric field, both at room temperature and at low temperature, on the photo-excited species by monitoring the photoluminescence (PL) yield and PL decays.

At room temperature (RT), we find that an applied electric field quenches the photoluminescence, as expected from field induced carrier separation and drift. However, we also find a significant reduction in the non-radiative monomolecular decay rate. The latter occurs on a slow (minutes) timescale, suggesting that mobile defects, which can drift under application of an electric field, are, at least in part, responsible for the non-radiative decay pathway.

We also performed the same experiment at 190K, in order to reduce the influence of temperature activated processes. We find that the radiative decay rate is greatly enhanced and we even observe evidence for rapid geminate recombination after the application of the electric field. The result is an increase in relative PLQY by up to 10 % after applying a field of 150 KV cm^{-1}. Combining these findings with electric field dependent Raman spectroscopy, we propose that the electric field induces an alignment and “locking” of the organic dipoles. This reduces their ability to screen the excited state Coulomb interactions and disrupts the electric fields within the polarized domains. The result is a strengthened electron – hole interaction. This work sheds new light on the crucial effect of the molecular dipole on electron – hole interactions in hybrid lead halide perovskites.

References

[1] Xiao, Z. *et al.* Giant switchable photovoltaic effect in organometal trihalide perovskite devices. *Nat Mater* .,Vol 14**,** (2015) 193–198.
[2] Snaith, H. J. *et al.* Anomalous Hysteresis in Perovskite Solar Cells. *J. Phys. Chem. Lett.* Vol 5, (2014), 1511-1515.
[3] Grancini *et al*. Role of microstructure in the electron-hole interactions of hybrid lead-halide perovskites, manuscript under revision.

[Talk#50]

Comprehensive Studies of New Schemes for Enhancing the Carrier Extraction and Light Absorption of Organic/Inorganic Solar Cells

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Carrier (electron and hole) transport layers (CTLs) are important components in organic optoelectronics such as organic solar cells (OSCs) and organic light emitting diodes (OLEDs), which can favor the efficient transport of carriers between the organic active layer and electrode as well as high optical transparency. Transition metal oxides are promising materials for CTLs because of their good electrical properties, stability, and optical transmission. We propose and demonstrate several low-cost approaches for forming transparent and efficient metal oxide-based carrier transport layers with the incorporation of metal nanoparticles [1,2]. The interesting features of the novel carrier extraction layers are low temperature (i.e. low cost), solution process (i.e. large area) and water free (i.e. compatible to most devices) for high performance optoelectronics [3]. With the knowledge of solution processed of organic and inorganic materials, we have recently proposed some new approaches such as vacuum-assisted thermal annealing of $CH_3NH_3PbI_3$ for highly stable and efficient perovskite SCs with power conversion efficiency (PCE) of 14.5% and no hysteresis [4]. Our latest theoretical prediction of PCE can reach 31% using the detailed balanced model.

Regarding light absorption of OSCs, a theoretical and experimental study of plasmonic OSCs with the metallic nanostructures is presented in this talk. From theoretical study, the physics of the performance enhancement of the organic solar cell is explained by multiphysics model of plasmonic OSCs. Meanwhile, we have also experimentally investigated the plasmo-optical [5] and plasmo-electrical [1,6,7] effects with various metallic nanostructures such as metallic nanoparticles and metallic nanogratings into different regions of the solar cells. Recently, by the new concept of plasmon-electrical effects, we break the space charge limit current of organic semiconductor which is a fundamental inherent property of organic semiconductor [7]. Our results show that the PCE of single junction OSCs can be enhanced by over 30% [8] and the value of PCE can reach about 9.62% [9] and the latest result can reach 10.5% depending on the metallic nanostructures, device structures, and the polymer materials. Details of the improvement will be discussed.

References

[1] *Adv. Funct. Mater.* Vol. 23, (2013), pp 4255-4261.
[2] *Energ. Environ. Sci.* Vol. 6, (2013), pp 3372-3379.
[3] *Adv. Mat.*, in press, DOI: 10.1002/adma.201405391; *Adv. Mat.*, vol. 25, (2013), pp 2051-2055; *Adv. Function. Mat.*, vol. 24, (2014), pp 7348-7356; *J. Mater. Chem. A*, vol. 1, (2013), pp 6614-6621.
[4] *ACS Nano*, vol. 9, (2015), pp 639-646.
[5] *Adv. Mat.*, vol. 26, (2014), pp 5368-5399.; *Scientific Reports*, vol. 5, (2015), pp 8525; *Adv. Mater.*, vol. 24, (2012) pp 3046-3052., *Adv. Funct. Mat.*, vol.23, (2013), pp 2728-2735.
[6] *Progress In Electromagnetics Research (PIER)*, invited, vol. 146, (2014), pp 25-46; *J. Mater. Chem.*, vol. 21, (2011), pp 16349-16356.
[7] *Scientific Reports*, vol. 4, (2014), pp 6236.
[8] *J. Mater. Chem.*, vol. 22, (2012), pp 1206-1211.
[9] Adv. Opt. Mat. DOI: 10.1002/adom.201500107.

[Talk#51]

Impact of Solvent Additive on Transport Properties and Photovoltaic Performance in Polymer:Fullerene Bulk-heterojunction System

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The morphological effects of solvent additive 1,8-diiodooctane (DIO) on bulk-heterojunction (BHJ) thin films for solar cells applications have been extensively studied by many research groups. However, studies on the influence of carrier mobilities on these films are still limited. In this work, we investigate both hole and electron transports in a state of the art polymer:fullerene system, namely PTB7:PC$_{71}$BM, by admittance spectroscopy. Interestingly, for a polymer:fullerene weight ratio of 1:1.5, the electron mobility in the blend film increases by two orders of magnitude with the DIO concentrations while almost no change is found in the hole mobility. The transport data reveal why the commonly used 3 vol% of DIO in this BHJ blend can achieve optimized solar cells. For a DIO concentration less than 3 vol%, the electron mobility is suppressed by large, but poorly connected PC$_{71}$BM domains. For a DIO concentration larger than 3 vol%, the electron mobility is improved drastically and the hole mobility becomes the limiting factor. Therefore, only at about 1.5 – 4 vol%, the electron and hole mobilities are in balance. The mobilities at different temperatures are analyzed by the Gaussian disorder model (GDM). We found that the DIO additive affects fundamentally the hopping distances of electrons. Our charge transport data suggest that there are alternative donor-acceptor ratios to achieve optimized the PTB7:PC$_{71}$BM based solar cells. We demonstrate that the fullerene content of the BHJ film can be significantly reduced from 1:1.5 to 1:1 while the optimized performance can still be preserved.

[Talk#52]

Multi-scale Modeling of Electronic Processes at the DTDCTB/C_{60} Interfaces for Organic Photovoltaics

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Electron transfer at the donor/acceptor interface is one of the key processes for conversion of light to electricity utilizing organic solar cells. We have carried out a multi-scale modeling on the exciton-dissociation and charge-recombination processes at the donor/acceptor interface for DTDCTB/C_{60} solar cells by means of molecular dynamics simulations and quantum-chemical calculations. Our calculated results reveal that high energy levels, namely “hot” charge-transfer states determine exciton dissociation in the DTDCTB/C_{60} complex for organic solar cells. In addition, molecular dynamics simulations show that the DTDCTB/C_{60} interface morphologies are much dependent on the structural characters of the DTDCTB substrate surface, such as stabilities, molecular arrangement patterns, and molecular orientations. Also, the interface morphologies can exert important impacts on the electronic processes in the DTDCTB/C_{60} solar cells.

References

[1] Yi Y., Coropceanu V., and Brédas J.-L., “Exciton-Dissociation and Charge-Recombination Processes in Pentacene/C60 Solar Cells: Theoretical Insight into the Impact of Interface Geometry”, *J. Am. Chem. Soc.*, Vol. 131, No. 43, (2009), pp 15777-15783.

[2] Lin L.-Y., Chen Y.-H., Huang Z.-Y., Lin H.-W., Chou S.-H., Lin F., Chen C.-W., Liu Y.-H., and Wong K.-T., “A Low-Energy-Gap Organic Dye for High-Performance Small-Molecule Organic Solar Cells”, *J. Am. Chem. Soc.*, Vol. 133, No. 40, (2011), pp 15822-15825.

[3] Muccioli L., D'Avino G., Zannoni C., “Simulation of Vapor-Phase Deposition and Growth of a Pentacene Thin Film on C_{60} (001)”, *Adv. Mater.*, Vol. 23, No. 39, (2011), pp 4532-4536.

[Talk#53]

Ultrafast Energy Dynamics in Biomimetic Nanoring Complexes

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Natural light-harvesting systems from photosynthetic bacteria are highly evolved for efficient energy collection, and their photophysics has been thoroughly investigated. Many of the photophysical features critical to their energy harvesting performance have been attributed to the geometrical structure of the key molecular complexes, namely LH1 and LH2. Photons captured by 'antenna' B800 chromophores generate excitons, which rapidly transfer to a ring motif composed of B850 chromophores. Many studies have highlighted the importance of the ring structure, which gives rise to unique features in energy funneling, state coherence, and delocalization.

We are intrigued by the possibility of creating synthetic biomimetic light-harvesting structures as a route to understanding (and potentially surpassing) the efficiency of natural systems. Through a combination of supramolecular chemistry and template-driven synthesis, we have produced antenna-nanoring complexes of porphyrin molecules [1]. By use of ultrafast time-resolved photoluminescence spectroscopy, we have found that the complexes exhibit efficient energy transfer between the antenna and nanoring molecules, with transfer rates of $(1.25\text{ps})^{-1}$ [1]. This rate is similar to that observed for naturally occurring LH2 complex. A powerful feature of this technique is that the synthetic approach allows for structures unseen in nature to be studied. By modifying the number of binding sites on the antenna molecule, a complex with two acceptor nanoring molecules was created, exhibiting an antenna to nanoring transfer rate of $(0.65\text{ps})^{-1}$.

Complete, ultrafast exciton delocalization on the B850 cycle in LH2 has been proposed to lend both state stability, enhanced overall efficiency and a reduced radiative rate to the natural light-harvesting system. To investigate the role of delocalization, we have studied photoluminescence properties of a range of large conjugated nanoring molecules [2,3]. Strikingly, we found superradiance effects (an increase in radiative rate with temperature) for nanorings, predicted but unseen in nature [2]. Ultrafast exciton delocalization enables superradiance, as it is indicative of a ground-state exciton which extends around the complete rim of the nanoring. We observe such delocalization for nanorings with an unprecedented size of up to 30 porphyrin units (around 10nm in diameter) [3]. Even beyond this size, significant differences persist in the nature of the emitting dipole polarization, arising from the topological difference between exciton migration on cyclic and linear changes.

The conjugated porphyrin nanoring platform provides a synthetic toolbox for studying some of the most interesting features in natural light-harvesting systems, from fundamental geometry-dependent exciton behavior [3], to superradiance [2], and as a model of complete light-harvesting systems [1].

References

[1] P. Parkinson, C. Knappke, N. Kamonsutthipajit, K. Sirithip, J. Matichak, H. Anderson and L. Herz, "Ultrafast Energy Transfer in Biomimetic Multistrand Nanorings", *JACS*, Vol. 136, (2014), pp 8217-8220

[2] C-K Yong, P. Parkinson, D. Kondratuk, W-H. Chen, A. Stannard, A. Summerfield, J. Sprakfe, M. O'Sullivan, P. Beton, H. Anderson and L. Herz, "Ultrafast delocalization of excitation in synthetic light-harvesting nanorings", *Chemical Science*, Vol. 6, (2015), pp. 181

[3] P. Parkinson, D. Kondratuk, C. Menelaou, J. Gong, H. Anderson and L. Herz, "Chromophores in Molecular Nanorings : When is a Ring a Ring?", *J Phys. Chem. Lett.*, Vol. 5, (2014), pp. 4356-4361

[Talk#54]

Ultrafast Broadband Photoluminescence Spectroscopy for Advanced Optoelectronic Materials

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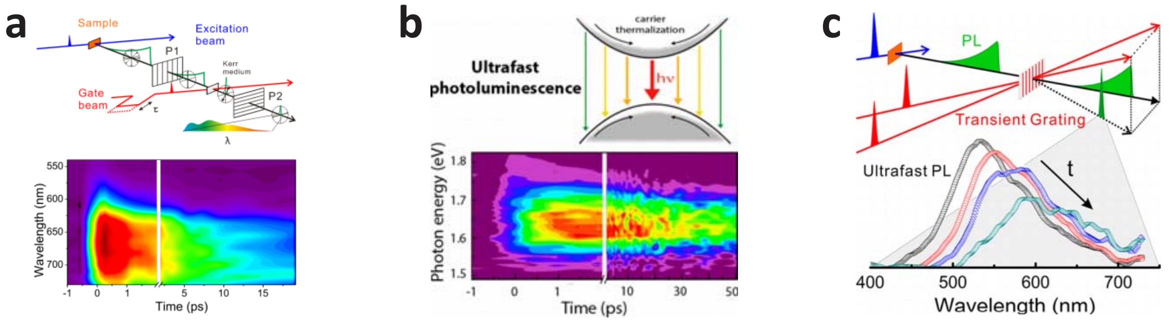
Time-resolved photoluminescence (TRPL) spectroscopy is a basic tool to probe photoexcitation dynamics in biosystems and advanced functional materials. To obtain rich information from TRPL spectra, ultrafast time resolution and broadband detection are desired. Recently, we have developed ultrafast TRPL spectroscopy techniques based on broadband phase matched third-order nonlinear optical gating and applied them to optoelectronic materials.

The TRPL system based on an optical Kerr gate shutter provides 200 fs time resolution and broad colour resolution in the visible to near infrared region. We first used this system to study ultrafast exciton dynamics in polymer photovoltaics (Fig. a).[1] From the amplitude of initial TRPL spectra of thin film samples, we can estimate the volume of initial excitation and correlate ultrafast charge carrier formation in polymer:fullerene blends to initially delocalized and non-relaxed excitations.

Next, we investigated the sub-picosecond TRPL dynamics in organometal halide perovskites (Fig. b).[2] From the picosecond rise time for PL and the lack of initial polarization anisotropy, we conclude that the PL dynamics are dominated by recombination of free charge carriers at room temperature. At high excitation fluence, we also resolved kinetics of amplified stimulated emission process as results of the kinetic interplay between carrier cooling and optical gain.

Finally, we present a novel TRPL technique, transient grating photoluminescence spectroscopy (Fig. c).[3] It features a compact setup, ultra-broad detection bandwidth (covering the whole visible region, and potentially beyond), ultrafast time resolution (200 fs) and extremely low background – a combination that outperforms other TRPL methods.



References

[1] Chen, K.; Barker, A. J.; Reish, M. E.; Gordon, K. C.; Hodgkiss, J. M. "Broadband Ultrafast Photoluminescence Spectroscopy Resolves Charge Photogeneration via Delocalized Hot Excitons in Polymer:fullerene Photovoltaic Blends." *J. Am. Chem. Soc.* 2013, 135, 18502–18512.

[2] Chen, K.; Barker, A. J.; Morgan, F. L. C.; Halpert, J. E.; Hodgkiss, J. M. "The Effect of Carrier Thermalization Dynamics on Light Emission and Amplification in Organometal Halide Perovskites" *J. Phys. Chem. Lett.* 2015, 6, 153–158.

[3] Chen, K.; Gallaher, J. K.; Barker, A. J.; Hodgkiss, J. M. Transient "Grating Photoluminescence Spectroscopy: An Ultrafast Method of Gating Broadband Spectra." *J. Phys. Chem. Lett.* 2014, 5, 1732–1737.

[Talk#55]

Structure-Directed Exciton Dynamics in Templated Porphyrin Nanorings

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Conjugated polymers with cyclic structures are interesting because their symmetry leads to unique electronic properties. Recent advances in Vernier templating[2] now allow large shape-persistent fully conjugated porphyrin nanorings to be synthesized, exhibiting unique electronic properties. We examine the impact of different conformations on exciton delocalization, transfer of electronic excitation and emission depolarization[1] in a range of different porphyrin nanoring topologies with comparable spatial extent.

Low photoluminescence anisotropy values are found to occur within the first few hundred femtoseconds after pulsed excitation for all nanorings, suggesting ultrafast delocalization of excitons across the nanoring structures[3]. Out-of-plane distortions associated with twisting and bending of the templated nanoring topologies cause further polarization memory loss[1] as indicated in Fig.1, which is supported by molecular dynamics simulations. Transfer of electronic excitation occurs for the nanotube (Fig. 2) from an initially formed state polarized in the direction of the nanotube axis (z-axis) to an excited state polarized in the x-y plane on the femtosecond timescale. As a result, a change of PL anisotropy from positive to negative values has been observed when tuning excitation wavelengths from Qx band (dipole moment in the x-y plane) more into Qy band (dipole moment along z-axis).

Fig. 1

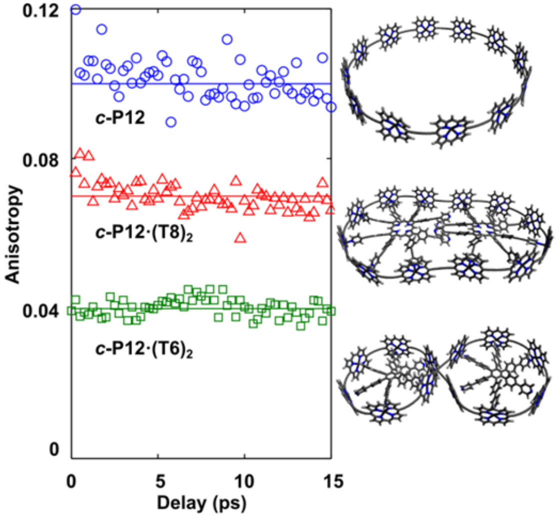
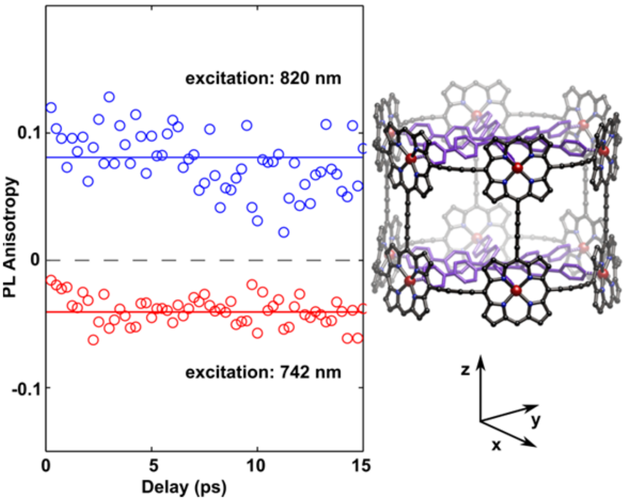


Fig. 2



References

[1] Gong J. Q., Parkinson P., Kondratuk D. V., Gil-Ramirez G., Anderson H. L. and Herz L. M., "Structure-Directed Exciton Dynamics in Templated Molecular Nanorings", *J. Phys. Chem. C,* 119, (2015), pp 6414-6420.

[2] Kondratuk D. V., Sprafke J. K., O'Sullivan M. C., Perdigao L. M., Saywell A., Malfois M., O'Shea J.N., Beton P.H., Thompson A.L. and Anderson H. L., "Vernier-Templated Synthesis, Crystal Structure, and Supramolecular Chemistry of a 12-Porphyrin Nanoring", *Chem. Eur. J.,* 20, (2014), pp 12826-12843.

[3] Yong C. K., Parkinson P., Kondratuk D.V., Chen W. H., Stannard A., Summerfield A., Sprafke J. K., O'Sullivan M. C., Beton P. H., Anderson H. L., Herz L. M., "Ultrafast Delocalization of Excitation in Synthetic Light-Harvesting Nanorings", *Chem. Sci.,* 6, (2015), pp 181-189.

[Talk#56]

Emerging Organic Optoelectronics Devices

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Organic LED (OLED) is the first successful organic optoelectronic device being made and it shows the way that organic materials can be used to fabricate practical optoelectronics. Its success has encouraged broader development of new organic materials and exploring new applications. In this presentation, we are presenting some of our recent works in applying new organic materials in new optoelectronic devices; this includes cascaded twin organic laser as vibrational sensor; optical pumped twin laser device was fabricated and its twin emission is calibrated to detect vibrational movement of the sensor. Using standard organic LED materials in TADF(Thermally Assisted Delayed Florescence) OLED device; appropriately selected donor and acceptor OLED materials were blended together to form the core energy re-harvesting layer for TADF process in the OLED. The emission performance increased by almost 5 times with the new design. Polymers with strong non-linear optical characteristic is being used as active medium for plasmonic device that can generate harmonics with optical spin Hall effect.

[Talk#57]

Multi-Molecular Conical Intersections in Ultrafast Singlet Exciton Fission

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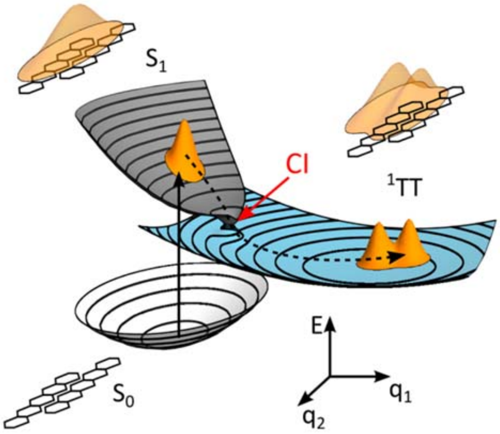
Singlet exciton fission is the process in organic semiconductors through which a spin-singlet exciton converts into a pair of spin-triplet excitons residing on different chromophores, entangled in an overall spin-zero state. For some systems, singlet fission has been shown to occur on the 100 fs timescale and with a 200% yield, but the mechanism of this process remains uncertain.[1,2] We study a model singlet fission system, TIPS-pentacene, using a novel ultrafast vibronic spectroscopy technique.[3] We observe that vibrational coherence in the initially photogenerated singlet state is transferred to the triplet state and show that this behaviour is effectively identical to that observed in ultrafast internal conversion for polyenes in solution.[4] This similarity in vibronic dynamics suggest that both multi-molecular singlet fission and single-molecular internal conversion are mediated by the same underlying relaxation processes, based on strong coupling between nuclear and electronic degrees of freedom. In its most efficient form this leads to a conical intersection between the coupled electronic states.



References

[1] Smith M. and Michl J., “Recent Advances in Singlet Fission”, *Annual Review of Physical Chemistry*, Vol. 64 (2013) pp 361-386.

[2] Yost S.R., Lee J., Wilson M.W.B., Wu T., McMahon D.P., Parkhurst R.R., Thompson N.J., Congreve D.N., Rao A., Johnson K., Sfeir M.Y., Bawendi M.G., Swager T.M., Friend R.H., Baldo M.A. and Voorhis T.V., “A transferable model for singlet-fission kinetics”, *Nature Chemistry*, Vol. 6, No. 6 (2014) pp492-497.

[3] Wende T., Liebel M., Schnedermann C., Pethick R. and Kukura P., “Population Controlled Impulsive Vibrational Spectroscopy: Background- and Baseline-Free Raman Spectroscopy of Excited Electronic States”, *The Journal of Physical Chemistry A*, Vol. 118, No. 43 (2014), pp 9976-9984.

[4] Musser A.J., Liebel M., Schnedermann C., Wende T., Kehoe T.B., Rao A. and Kukura P., “Evidence for Conical Intersection Dynamics Mediating Ultrafast Singlet Exciton Fission”, *Nature Physics*, Vol. 11 (2015), in press.

[Talk#58]

Optically-pumped Lasing and Hot Phonon Bottleneck in Mixed Halide Perovskite Photovoltaic Semiconductors

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Organometallic mixed halide perovskite-based solar cells have shown a breakthrough in power conversion efficiency [1,2] with power conversion efficiencies recently exceeding 20% [3]. To rationalize the origin of the high efficiencies, we investigate the recombination mechanism and fundamental nature of photoexcitations in these novel materials. Since charge modulating devices are not available, we use transient spectroscopy to extract charge carrier parameters such as carrier cooling times and the effective mass, which give insights on transport properties.

We report the transient photoluminescence and transient absorption of photovoltaic devices and spin-coated perovskite films in the range from 30 fs to several microseconds. We find that free charge carrier generation in pristine $CH_3NH_3PbI_{3-x}Cl_x$ perovskite occurs within 1 ps, and that these free charge carriers undergo bimolecular recombination on timescales of 10s to 100s of nanoseconds, to give photoluminescence with quantum efficiency above 50%. To exemplify the high luminescence yield of $CH_3NH_3PbI_{3-x}Cl_x$ perovskites, we construct and demonstrate the operation of the first optically-pumped vertical laser cavity with a layer of perovskite as the gain medium [4]. We note that these long carrier lifetimes together with exceptionally high luminescence yield are unprecedented in such simply prepared inorganic semiconductors and that these properties are ideally suited for photovoltaic diode operation [5].

We use ultrafast transient absorption (TA) spectroscopy to study hot carrier distributions and quantify key semiconductor parameters. Above-bandgap, non-resonant excitation creates quasi-thermalized carrier distributions within 100 fs. During carrier cooling, a sub-bandgap TA signal arises at 1.58 eV, which is explained by the interplay of band-gap renormalization and hot carrier distributions. At higher excitation densities, carrier cooling is substantially slowed due to a ‘phonon bottleneck’. The appearance of this effect indicates low impurity and phonon-phonon scattering in these polycrystalline materials, which contributes to high charge carrier mobilities. Using a simple band-filling model that accounts for photoinduced reflectivity changes, we determine a small effective mass of $m_r = 0.14\ m_e$, which agrees with band structure calculations and high photovoltaic performance.

References

[1] Lee, M. M., Teuscher, J., Miyasaka, T., Murakami, T. N. & Snaith, H. J. Efficient Hybrid Solar Cells Based on Meso-Superstructured Organometal Halide Perovskites. Science 338, (2012), 643-647

[2] H. S. Kim, C. R. Lee, J. H. Im, K. B. Lee, T. Moehl, A. Marchioro, S. J. Moon, R. Humphry-Baker, J. H. Yum, J. E. Moser, M. Gratzel, N. G. Park, Scientific reports 2012, 2, 591.

[3] NREL, Efficiency Chart, http://www.nrel.gov/ncpv/images/efficiency_chart.jpg

[4] F. Deschler, M. Price, S. Pathak, L. E. Klintberg, D.-D. Jarausch, R. Higler, S. Hüttner, T. Leijtens, S. D. Stranks, H. J. Snaith, M. Atatüre, R. T. Phillips, R. H. Friend, The Journal of Physical Chemistry Letters 2014, 5, 1421.

[5] Miller, O. D., Yablonovitch, E. & Kurtz, S. R. Strong Internal and External Luminescence as Solar Cells Approach the Shockley-Queisser Limit. Photovoltaics, IEEE Journal of 2, (2012), 303-311

[Talk#59]

Aggregation and Morphology Control Enables Multiple Cases of High-efficiency Polymer Solar Cells

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Although the field of polymer solar cell has seen much progress in device performance in the past few years, several limitations are holding back its further development. For instance, current high-efficiency (>9.0%) cells are restricted to materials combinations that are based on limited donor polymers and only one specific fullerene acceptor. Here we report the achievement of high-performance (efficiencies up to 10.8%, fill factors up to 77%) thick-film polymer solar cells for multiple polymer:fullerene combinations via the formation of a near-ideal polymer:fullerene morphology that contains highly crystalline yet reasonably small polymer domains. This morphology is controlled by the temperature-dependent aggregation behavior of the donor polymers and is insensitive to the choice of fullerenes. The uncovered aggregation and design rules yield three high-efficiency (>10%) donor polymers and will allow further synthetic advances and matching of both the polymer and fullerene materials, potentially leading to significantly improved performance and increased design flexibility.

References

[1] Y. Liu, J. Zhao, Z. Li, C. Mu, W. Ma, H. Hu, K. Jiang, H. Lin,H. Ade and H. Yan, “Aggregation and morphology control enables multiple cases of high-efficiency polymer solar cells”, *Nature Communications*, Vol. 5, (2014), pp 5293.

[Talk#60]

A Multiscale Simulation Framework for Novel Photovoltaic Materials

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The overall photovoltaic process in various novel materials is a typical multiscale interaction issue, thus the device performance is controlled by a series of complicated phenomena that span a range of length and time scales. As a consequence, only those theoretical simulation methods with multiscale characteristics can fully and efficiently describe the photovoltaic mechanism in those emerging solar cells. In this abstract we present a new hybrid quantum mechanics and electromagnetics (QM/EM) method to study the interaction between charge and electromagnetic field in novel optoelectronic devices and materials.

In the QM/EM method, the regions of the system where active electron scattering processes take place are treated quantum mechanically, while Maxwell's equations and a semi-classical drift-diffusion model are coupled to describe the surroundings. The QM and EM models are solved, respectively, in different regions of the system in a self-consistent manner. Potential distributions and current densities at the interface between QM and EM regions are employed as the boundary conditions for the quantum mechanical and electromagnetic simulations, respectively.

Before applying this multiscale scheme to photovoltaic devices, we analyzed the accuracy and efficiency of the QM/EM method by simulations of a carbon nanotube-based molecular device. We simulated the optical response of a tandem photovoltaic cell and demonstrated that multiple QM regions are coupled through the classical EM model. We also investigated plasmon-inducing effects for enhanced photovoltaic conversion by extending the static QM/EM method to the time- and frequency-domain for dynamic properties. The QM/EM model is further expected to describe several complicated optoelectronic systems, like organic solar cells.

References

[1] Meng L., Shang Y., Li Q., Li Y., Zhan X., Shuai Z., Kimber R. G. E. and Walker A. B., "Dynamic Monte Carlo Simulation for Highly Efficient Polymer Blend Photovoltaics", *J. Phys. Chem. B*, Vol. 114, (2010), pp 36-41.

[2] Meng L., Wang D., Li Q., Yi Y., Bredas J.-L. and Shuai Z., "An improved dynamic Monte Carlo model coupled with Poisson equation to simulate the performance of organic photovoltaic devices", *J. Chem. Phys.*, Vol. 134, (2011), pp 124102.

[3] Yam C., Meng L., Chen G. H., Chen Q. and Wong N., "Multiscale Quantum Mechanics/Electromagnetics Simulation for Electronic Devices", *Phys. Chem. Chem. Phys.*, Vol. 13, (2011), pp 14365.

[4] Meng L., Yam C., Koo S., Chen Q., Wong N., and Chen G. H., "Dynamic Multiscale Quantum Mechanics/Electromagnetics Simulation Method", *J. Chem. Theory Comput.*, Vol. 8, (2012), pp 1190.

[5] Meng L., Yin Z., Yam C., Koo S., Chen Q., Wong N., and Chen G., "Frequency-domain multiscale quantum mechanics/electromagnetics simulation method", *J. Chem. Phys.*, Vol. 139, (2013), pp 244111.

[6] Yam C., Meng L., Zhang Y., and Chen G., "A multiscale quantum mechanics/electromagnetics method for device simulations", *Chem. Soc. Rev.*, Vol. 44, (2015), pp 1763-1776.

[Talk#61]

Mapping Photoinduced Ionic Migration and Segregation in Mixed-halide Hybrid Perovskites

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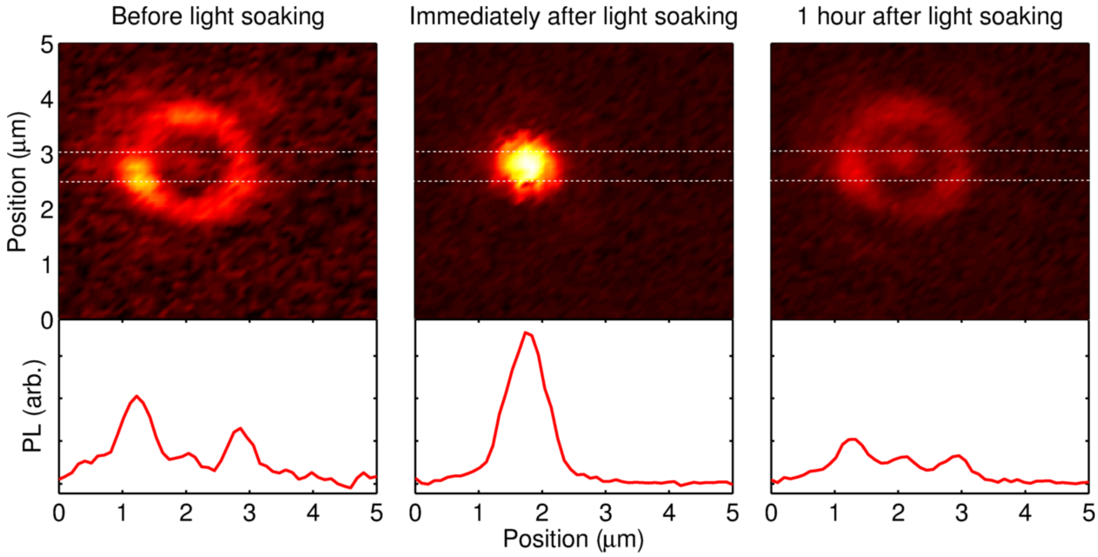
Organo-metal halide perovskites (such as $CH_3NH_3PbI_3$) have recently attracted huge interest, with potential use as a solution processable semiconductor for photovoltaics, LEDs and lasers. Of particular appeal is the ability to continuously tune the bandgap over a wide range by blending different halides (Cl, Br or I) in to the structure in various ratios.[1] However, the emergence of a strong sub-bandgap photoluminescence feature after light soaking[2] implies that stability is of concern in these mixed-halide perovskites. The emergence of this feature is completely reversible (on timescales of minutes), and while its origin is not entirely clear, photo-induced splitting of XRD peaks suggests halide segregation.[2] Interestingly, the feature is always at 740 nm, independent of initial sample bandgap.

By collecting maps of PL and transmission spectra through a confocal microscope, we show that the sub-bandgap emission in mixed iodide-bromide perovskites originates in localized regions of enriched iodide concentration. Furthermore, we show that these features change shape upon light soaking, so as to further increase the local iodide concentration. This may be the strongest evidence to date that ion migration takes place in organo-metal halide perovskites.

Finally, we use femtosecond transient absorption spectroscopy to resolve the transfer of charges from the majority phase to the photoinduced iodide-rich phases over tens of picoseconds. The iodide-rich phases act as luminescent traps, explaining how they can dominate the bulk PL spectra even in cases where they comprise only a small fraction of the total material.



References

[1] Noh, J. H., Im, S. H., Heo, J. H., Mandal, T. N. & Seok, S. Il. "Chemical management for colorful, efficient, and stable inorganic-organic hybrid nanostructured solar cells". *Nano Lett.* **13,** (2013).

[2] Hoke, E. T. *et al.* Reversible photo-induced trap formation in mixed-halide hybrid perovskites for photovoltaics. *Chem. Sci.* **6,** 613–617 (2015).

[Talk#62]

Bimolecular Nature of Fluence Dependent Radiative Recombination Processes in Hybrid Lead Bromide and Iodide Perovskites

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Organometallic halide perovskites have been established in the field of optoelectronics due to their use in efficient photovoltaic devices, with conversion efficiencies recently reaching 20% [1]. Emerging promising applications of these materials have been demonstrated in LEDs and optically pumped LASERs. However, the success of these novel applications depends on achieving high photoluminescence quantum efficiencies (PLQE), which are defined by the ratio between radiative and non-radiative decay channels. It is therefore crucial to understand the interplay between different recombination mechanisms and the effect of material composition on the nature of photo-excitations.

In our work, we investigate the recombination of photo-excited charge carriers in methylammonium lead bromide and iodide perovskites (CH3NH3PbX3, X=Br,I) using transient absorption (TA) and photoluminescence (PL) spectroscopy in the time range of 100 fs to 100s of nanoseconds.

We find fluence dependent recombination kinetics in iodide and bromide perovskite, which indicates that different recombination mechanisms dominate depending on excitation density. Consistent with previous reports[2], we find that the radiative recombination mechanism in iodide perovskite is bimolecular at excitation densities from 10^{14} to $10^{18}/\mathrm{cm}^3$. PL kinetics of bromide perovskites, however, show mono-exponential behaviour. By combining TA and PL data, and thus separating radiative from non-radiative components, we demonstrate that radiative recombination in bromide perovskites is also bimolecular. However, since non-radiative monomolecular decay channels are dominant in bromide perovskite, the overall kinetics are mono-exponential. This point towards a non-excitonic nature of the photoexcited states in bromide perovskites. We find recombination rates which are one order of magnitude larger for bromide than for iodide perovskite. For the first time, we observe Auger type kinetics at fluences $> 10^{18}/\mathrm{cm}^3$ which sets a fundamental limit for the use of these materials in LASERs and LEDs.

References

[1] http://www.nrel.gov/ncpv/images/efficiency_chart.jpg
[2] Deschler, F. *et al.* High Photoluminescence Efficiency and Optically Pumped Lasing in Solution-Processed Mixed Halide Perovskite Semiconductors. *J. Phys. Chem. Lett.* **5,** 1421–1426 (2014).

[Talk#63]

Defect Engineering and the Enhancement of The Power Conversion Efficiency of Perovskite based Solar Cells

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We report experimental investigation of the fabrication and characterization of perovskite based solar cells. Systematic investigation of the influences of post-deposition thermal annealing in oxygen ambient on the performance of solution-processed $CH_3NH_3PbI_3$-based planar solar cells. Detailed investigation of photothermal deflection spectroscopy on $CH_3NH_3PbI_3$ films deposited on quartz substrates with systematically varied deposition and annealing parameters.[1,2] The experimental results clearly demonstrated significant reduction in the bandgap states arising from O_2 annealing as shown in Fig. 1. Complete photovoltaic devices were fabricated on planar TiO_2 as the electron transport layer and spiro-MeOTAD as the hole transport layer. Significant increase in the power conversion efficiencies (PCEs) of the devices were observed, as shown in Fig. 2, with an optimal annealing temperature of 65°C. Strong dependence on the annealing temperature for the PCEs of the devices suggests that a thermally activated process may underlie the observed phenomenon. Our experimental data indicate that O_2 treatments may result in substantially reduced trap density in the device and thereby significantly improving the lifetimes of the carriers.

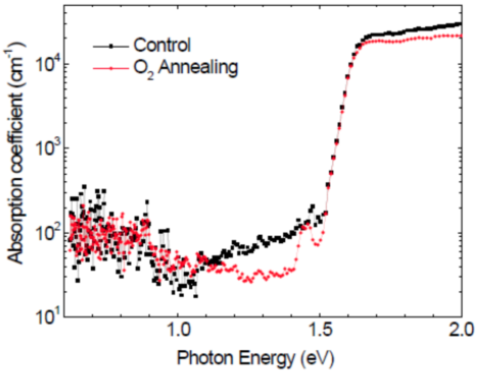

Fig. 1: Experimental PDS data for an O_2 annealed sample and the control.

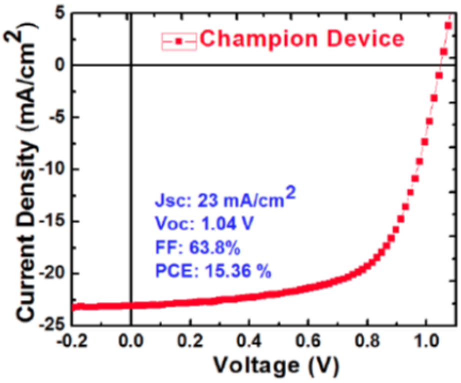

Fig. 2: The light *I-V* characteristics of a device annealed in O_2 ambient.

References

[1] Z. W. Ren, A. Ng, Q. Shen, H. C. Gokkaya, J. C. Wang, L. J. Yang, W. K. Yiu, A. B. Djurišić, W. W. F. Leung, W. K. Chan and C. Surya, "Thermal Assisted Oxygen Annealing for High Efficiency Planar $CH_3NH_3PbI_3$ Perovskite Solar Cell" Scientific Reports Vol. 4, (2014) pp. 6752;

[2] A. Ng, Z. W. Ren, Q. Shen, H. C. Gokkaya, G. X. Bai, J. C. Wang, L. J. Yang, A. B. Djurišić, W. W. F. Leung, J. H. Hao, W. K. Chan and C. Surya, "Efficiency enhancement by defect engineering in perovskite photovoltaic cells prepared by evaporated PbI_2/CH_3NH_3I multilayers", *Journal of Materials Chemistry A*, 2015.

[Talk#64]

Local Versus Long-Range Diffusion Effects of Photoexcited States on Radiative Recombination in Organic-Inorganic Lead Halide Perovskites

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Hybrid lead halide perovskites have been demonstrated as promising materials for highly efficient photovoltaic [1] and light-emitting optoelectronic applications [2]. The observation of long excited state lifetimes and high radiative bimolecular recombination efficiencies indicates very promising semiconducting properties [3,4]. In order to rationalize and optimize the operation of devices, an understanding of the microscopic recombination mechanisms of photoexcitations in these poly-crystalline materials is necessary.

Here, we study the spatial emission of the archetypical, high-performing perovskites $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ with high spatial and temporal emission. We use scanning near-field optical microscope (SNOM) in order to achieve excitation resolution <150 nm. Photoluminescence (PL) is collected in confocal geometry with ~300nm resolution and spectra are detected with a CCD. PL decays are recorded during spatial scans using time-correlated detection.

We report that radiative recombination in thin films (thickness <300 nm) of hybrid perovskite materials shows localized regions of increased emission with dimensions as low as 200 nm. The excited state lifetime in these high emission regions is increased and quantitatively follows the spatial intensity variation. Surprisingly, regions of high emission intensity are not affected by nearby regions with faster non-radiative decays. Excited states do not diffuse out of high emission regions before they decay, but are decoupled from nearby regions, either by slow diffusion rates or energetic barriers, which can be associated with structural/grain boundaries. Maps of the spectral emission line shape show narrower emission lines in high emission regions, which we attribute to increased order and possibly as areas of enhanced material quality and increased crystallinity. The expansion of the observed high emission regions to larger areas of the film raises the prospect to further increase the reported high PLQE values [3] (~20% - $CH_3NH_3PbBr_3$, ~50% - $CH_3NH_3PbI_3$) and to fabricate materials and devices with vastly increased optoelectronic performance.

References

[1] Lee, M. M., Teuscher, J., Miyasaka, T., Murakami, T. N. & Snaith, H. J., "Efficient Hybrid Solar Cells Based on Meso-Superstructured Organometal Halide Perovskites", *Science* **338**, (2012), 643-647, doi:10.1126/science.1228604

[2] Tan, Z. K. *et al.,* "Bright light-emitting diodes based on organometal halide perovskite", *Nature nanotechnology* **9**, (2014), 687-692, doi:10.1038/nnano.2014.149

[3] Deschler, F. *et al.,* "High Photoluminescence Efficiency and Optically Pumped Lasing in Solution-Processed Mixed Halide Perovskite Semiconductors", *The Journal of Physical Chemistry Letters* **5**, (2014), 1421-1426, doi:10.1021/jz5005285

[4] Stranks, S. D. *et al.,* "Electron-Hole Diffusion Lengths Exceeding 1 Micrometer in an Organometal Trihalide Perovskite Absorber", *Science* 342, (2013), 341-344, doi:10.1126/science.1243982

[Talk#65]

Photoconductive Cathode Interlayer for Highly Efficient Inverted Polymer Solar Cells

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Cathode interlayer between the active layer and conductive electrode plays a key role for the performance of organic solar cells due to its fundamental importance to the electron extraction process. Herein, we demonstrate that a highly photoconductive cathode interlayer can be achieved by doping 1wt% light absorber, i.e. perylene bisimide (PBI), into Zinc oxide (ZnO) thin film, which absorbs a very small amount of light but shows highly increased conductivity of 4.5×10^{-3} S/m under sunlight. The photovoltaic devices based on this kind of photoactive cathode interlayer exhibit significantly improved device performance, which is rather insensitive to the thickness of the cathode interlayer over a broad range. Moreover, a power conversion efficiency (PCE) as high as 9.6% was obtained by incorporation of our photoactive thin film with the classical PFN as a double-layer cathode inter-layer in the device using the blend of PTB7: $PC_{71}BM$ as the active layer, which is one of the best results in PTB7- based devices.[1]

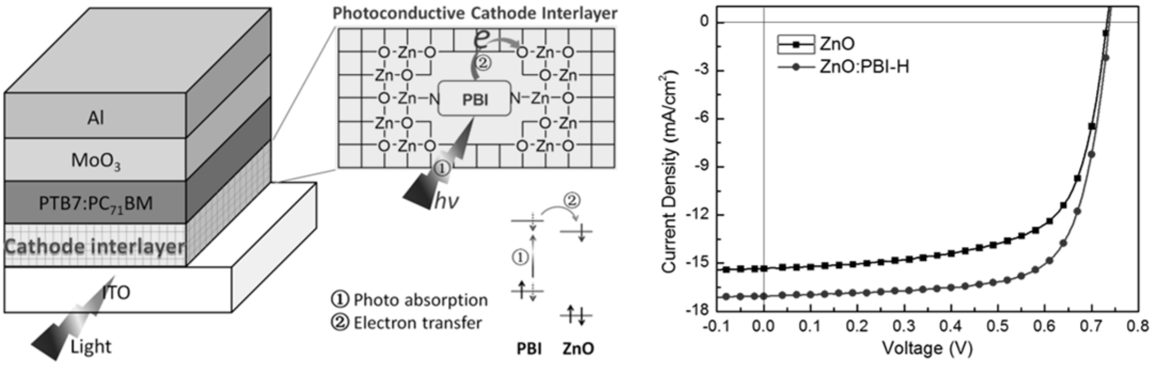

Fig. 1. Left: Schematic of photoconductive cathode interlayer in inverted polymer solar cells (i-PSCs). Right: J-V characteristics of the i-PSCs under 1000W/m^2 AM 1.5G illumination.

References

[1] Nian L., Zhang W. Q., Zhu N., Liu L. L., Xie Z. Q., Wu H. B., Würthner F., Ma Y. G., “Photoconductive Cathode Interlayer of Perylene Bisimide Doped Zinc Oxide for Highly Efficient Inverted Polymer Solar Cells”, *Journal of the American Chemical Society*, In revision (2015).

[Talk#66]

Anisotropic Carrier Thermalisation and Morphology-dependent Polarisation Memory in Organometallic Halide Perovskites

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Organometallic halide perovskites are at the frontier of optoelectronic research due to their excellent semiconductor properties and solution processability. We use ultrafast polarisation selective transient absorption spectroscopy (TA) to establish how the properties of excited states in these hybrid perovskite materials are determined by the interplay between their disordered macrostructure and local highly-crystalline domains.

It has been shown that $CH_3NH_3PbI_3$ perovskite films exhibit long-lived polarisation memory on 100s of picosecond timescales[1,2] but the origin of the anisotropy and its ultrafast behaviour are not well understood. We resolve the ultrafast process of carrier thermalisation in $CH_3NH_3PbI_3$ films using broadband TA with ~30 fs time resolution. We find that both the ultrafast spectral response and thermalisation rates show a large polarisation anisotropy, which depends strongly on carrier density. The observation of such non-thermalised, hot carrier populations enables us to investigate the dissipative mechanisms of carrier-carrier and carrier-phonon scattering. We also measure the decay of the long lived polarisation memory and use these results to examine how polarisation loss and charge carrier recombination depends on crystal size and materials processing. These insights into the polarisation memory and fundamental semiconducting properties of hybrid perovskites will help to guide the development of future photovoltaic devices, LEDs and electrically pumped lasers made from these materials.

References

[1] Sheng C. et al., “Exciton versus Free Carrier Photogeneration in Organometal Trihalide Perovskites Probed by Broadband Ultrafast Polarization Memory Dynamics”, *Phys. Rev. Lett.*, Vol. 114, No. 11, (2015), pp 1-5.

[2] Giovanni D. et al., “Highly Spin-Polarized Carrier Dynamics and Ultralarge Photoinduced Magnetization in CH3NH3PbI3 Perovskite Thin Films”, *Nano Lett.*, Vol. 15, No. 3, (2015), pp 1553-1558.

[Poster#01]

Luminescence Enhancement in Dinuclear Alkynylplatinum(II) Complexes Driven by Hierarchical Assembly Through Pt···Pt and π–π Stacking Interactions

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A luminescent dinuclear alkynylplatinum(II) complex containing an amphiphilic binaphthol bridge was designed and synthesized, and was shown to display cylindrical columnar assemblies in aqueous acetonitrile solutions, presumably mediated by the Pt···Pt and π–π stacking interactions. The length of the binaphthol bridge was found to have a profound effect on the degree of helicity for hierarchical helices of helices and serves as a critical determinant in the formation of tertiary structures for foldamers. Interestingly, the reciprocal association of multiple helices has led to luminescence enhancement behavior, which provides a luminescence turn-on switch for the reporting of the hierarchical assembly of foldamers into higher-order structures, distinct from that of the pure organic systems. Such a transverse aggregation of multiple helices driven by metallophilic interactions has been studied by electronic absorption, circular dichroism, emission spectroscopy and electron microscopy.

References

[1] S. Y.-L. Leung, A. Y.-Y Tam, C. H. Tao, H. S. Chow, V. W.-W. Yam *J. Am. Chem. Soc.* **2012**, *134*, 1047–1056.
[2] S. Y.-L. Leung, W. H. Lam, V. W.-W. Yam *Proc. Natl. Acad. Sci. USA* **2013**, *110*, 7986–7991.
[3] S. Y.-L. Leung, V. W.-W. Yam *Chem. Sci.* **2013**, *4*, 4228–4234.

[Poster#02]

Synthesis and Photo-Induced Electron Injection Process Studies in a Ruthenium Containing Triblock Copolymer/Multi-Walled Carbon Nanotubes Composite

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In this project, new photoactive ABA triblock copolymers incorporated with pyrene and ruthenium terpyridyl complex moieties were synthesized by reversible addition−fragmentation chain transfer polymerization. The molecule was also confirmed by GPC and ^{1}H NMR. The pyrene block in the copolymer can disperse and functionalize muti-walled carbon nanotubes (MWCNTs) by non-covalent π-π interaction to prepare the polymer/MWCNT composites. The ruthenium complex was widely used as photosensitizers and it greatly enhanced the photosensitivity of the functionalized nanotubes in the visible region compared to the pure nanotubes. The polymer/MWCNT composites were characterized by TEM, and UV-visible absorption. Cyclic voltammetry results showed that after photoexcitation of the ruthenium complexes, electron transfer from the sensitizer to carbon nanotubes may occur. In order to further understand the electronic interactions between the metal complex and the CNT surface, the charge generation and the transport dynamics of both pure polymers and composite were monitored by femto- and nano- second transient absorption (TA) spectroscopy. It was found that the lifetime of the excited state of the composite was much shorter than that of pure polymers. According to the decay dynamics at 571nm, it was observed that there is strong electronic interaction between the metal containing polymers and carbon nanotubes. This study about the electron injection process between polymeric sensitizers and carbon nanotubes can help in the development of device design based on polymer/CNT composites.

[Poster#03]

Twisting Donor-acceptor-donor Type Pyridine Derivatives: The Synthesis and Photophysical Investigations of Intramolecular Charge Transfer State

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In this work, a novel series of donor-acceptor-donor (D-A-D) type structured pyridine derivatives were synthesised and detailed photo-physical investigations were reported using steady-state and time-resolved spectroscopy techniques at varying temperatures. The investigations showed that the molecules have solvent polarity and temperature dependent excited-state configurations which was confirmed in two different polarity solvents (295-90 K), e.g. methyl cyclohexane (MCH) and 2-methyltetrahdrafuran (2-MeTHF). In MCH, a remarkable investigation of the molecules was observation of the dual fluorescence phenomena over the temperature range of 295-90K. At 295 K, the ground-state configuration of the molecules has planar geometry, therefore, the emission originates totally from locally excited (LE), however once the temperature is lowered to 90K, the molecular configuration showed structural reorganization, hence, the emission has the origin of fully-relaxed intramolecular charge transfer states (ICT), which can be attributed to the temperature effect upon excited-state molecular configuration as formation of ICT states. In particular, the ICT excited-states have different molecular configurations due to the presence of diffenent electron-donoting groups, e.g. the molecule including anthracene groups has 90^0 twisted geometry and triphenylamine including molecule has wagged geometrical folding, therefore, the decrease in temperature results in an enhancement in donor degree of rotations. Furthermore, one of the intriguing fluorescene spectrum behaviour was observed with the molecules in 2-MeTHF solution in the range of 295-90 K. In particular, the fluorescence spectrum gradually red-shifts through the fluid to glass transition temperature (~135 K), in this case, the fluorescence has taken place after full solvent-relaxations, but then, upon cooling the temperature (<135 K), the spectra dramatically shifted to blue and start emitting from LE excited-states. This significant change in the nature of the emitting spaces was explained with specific solvent-solute interactions in the vicinity of solvation dynamics. Finally, we have confirmed that the molecules have ICT ground-state geometry in solid-state phases (spin-coated films). And the decay dynamics were investigated comparing with the spin-coated films (at RT and 25 K) and MCH solutions (at 295K and 90 K).

[Poster#04]

Realization of the Population Inversion in a Conjugated Polymer by a Single or Double Stimulating Pulse

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By applying a single or double stimulating pulse to a conjugated polymer, we theoretically realize the population inversion between the corresponding intragap states. The simulations are performed within the framework of an extended version of the one-dimensional Su–Schrieffer–Heeger tight-binding model combined with a nonadiabatic evolution method. In the discussions, we mainly compare the stimulating intensity thresholds between the two different pumped modes, at which the population inversion in the polymer is reached. It is found that, the stimulating intensity threshold can be remarkably reduced by employing a double stimulating pulse rather than a single one. Effect of the lasting time for each pulse on the threshold is also discussed. We then propose a new optical-pumped mode to realize the population inversion in a polymer, which is potentially of great importance for polymer lasers.

References

[1] Samuel I. D. W., and Turnbull G. A., "Organic Semiconductor Lasers", *Chem. Rev*., Vol. 107, No. 4, (2007), pp 1272-1295.

[2] Gao K., Xie S. J., Yin S., and Liu D. S., "Biexcitons generation in a polymer by a femtosecond electric pump pulse", *Organic Electronics*, Vol. 13, No. 5, (2012), pp 784-788..

[3] Gao K., Xie S. J., Li Y., and Xia C. J., "Realization of the population inversion in a conjugated polymer by a single or double stimulating pulse", *Organic Electronics*, Vol. 15, No. 9, (2014), pp 1965-1971.

[Poster#05]

Tuning the Singlet–triplet Energy Gap of AIE Luminogens: Crystallization-induced Room Temperature Phosphorescence and Delay Fluorescence, Tunable Temperature Response, Highly Efficient Non-doped OLEDs

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In this contribution, we finely tuned the singlet–triplet energy gap (ΔE_{ST}) of luminescent materials with aggregation-induced emission (AIE) characteristics to modulate their fluorescence, phosphorescence and delay fluorescence via rational molecular design and investigated the possible ways to harvest their triplet energy in non-doped organic light-emitting diodes (OLEDs). Noteworthily, two molecules *o*-TPA-3TPE-*o*-PhCN and *o*-TPA-3TPE-*p*-PhCN with larger ΔE_{ST} values (0.59 eV and 0.45 eV, respectively) emitted efficient long-lived low temperature phosphorescence in their glassy solutions and exhibited efficient crystallization-induced room temperature phosphorescence. Meanwhile, it was the first time to observe a novel crystallization-induced delay fluorescence phenomenon in another AIE-active molecule *p*-TPA-3TPE-*p*-PhCN owing to its very small ΔE_{ST} value (0.21 eV). It was also found that molecules with various ΔE_{ST} values showed significantly different temperature sensitivity. Non-doped electroluminescent devices using these molecules as the single light-emitting layers were fabricated, exhibiting external quantum efficiencies higher than theoretical values of purely singlet emitter type devices. Particularly, *p*-TPA-3TPE-*p*-PhCN showed outstanding device performances with high luminance and efficiencies up to 36 900 cd m^{-2}, 11.2 lm W^{-1}, 12.8 cd A^{-1} and 4.37%, respectively, considering that its solid-state quantum yield was only 42%. All the above observations suggested that tuning the ΔE_{ST} values of AIE materials is a powerful methodology to generate many more interesting and meaningful optoelectronic properties.

Reference

[1] Li J., Jiang Y., Cheng J., Zhang Y., Su H., Lam J.W., Sung H.H., Wong K.S., Kwok H.S., and Tang B.Z., "Tuning the singlet-triplet energy gap of AIE luminogens: crystallization-induced room temperature phosphorescence and delay fluorescence, tunable temperature response, highly efficient non-doped organic light-emitting diodes", *Phys. Chem. Chem. Phys.*, Vol. 2, No. 17, (2005), pp 1134-1141.

[Poster#06]

Two-photon Optical Properties of AIE-active D-TPE-A Molecules: Aggregation Enhancement and Structure-Property Relationships

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We present an aggregation enhancement in two-photon-excited fluorescence (TPEF) of about two orders of magnitude in a series of novel non-centrosymmetric D-π-A molecules. Aggregation-induced emission property is introduced into these D-π-A molecules via tetraphenylethylene (TPE), which is served as their π-bridge. Detailed analysis shows that the TPEF of these molecules are enhanced in aggregation environment with both reinforcements in fluorescence quantum efficiency and two-photon absorptivity concomitantly. For each compound, the aggregation enhancement in fluorescence quantum efficiency is due to the restriction of intramolecular rotation upon aggregation that reduce the non-radiative decay rate upon excitation.[2] The aggregation enhancement in two-photon absorption (TPA) may attribute to the conformational change. For example, the free rotation of the conjugated chains is restricted so that the electronic communication is improved, and the planarization of the TPE structure further prolong the π-electron conjugation.[3] The TPA transition bands of these branched- or butterfly-configured molecules are similar to those in their linear absorption. The molecular TPA cross sections in aggregation environment reach around 50-130 GM, and peak within the available wavelength ranges of a Ti: Sapphire femtosecond oscillator. We also observe that two-photon absorptivity increases progressively with the addition of more donor/acceptor moieties on the TPE backbone. This phenomenon is presumably attributed to the improved conjugation length and enhanced intramolecular charge transfer, hence better delocalization of π-electrons.

References

[1] Zhang, Y.,Li, J.,Tang, B. Z.,Wong, K. S. "Aggregation Enhancement on Two-Photon Optical Properties of AIE-Active D-TPE-A Molecules". *J. Phys. Chem. C.* Vol. 118, No. 46, (2014), pp 26981-26986.

[2] Hong, Y. N.,Lam, J. W. Y.,Tang, B. Z. "Aggregation-Induced Emission: Phenomenon, Mechanism and Applications". *Chem. Commun.* Vol. 0, No. 29, (2009), pp 4332-4353.

[3] Pawlicki, M.,Collins, H. A.,Denning, R. G.,Anderson, H. L. "Two-Photon Absorption and the Design of Two-Photon Dyes". *Angew. Chem. Int. Ed. Engl.* Vol. 48, No. 18, (2009), pp 3244-3266.

[Poster#07]

Spectroscopic Studies of Different Poly3hexylthiophene Chain Environments in a Polyfluorene Matrix

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Polythiophenes are known to show complex morphology, and mixing them with a host such as polyfluorene could potentially exhibit complex photophysical behavior arising from complex energy transfer channels. However, controlling energy transfer processes is a difficult task because it depends on the interfaces between the two materials and their relative amounts. A blend composed of polyfluorene and thiophene may allow us to understand the underlying mechanisms of inter/intramolecular interaction of these two classes of materials.

Optical properties of blends made of Poly(9,9-dioctyl-fluorene-2,7-diyl) (PFO) and Poly(3-hexylthiophene-2,5-diyl) (P3HT) were investigated and compered to Poly(9,9-dioctylfluorene-alt-bithiophene) (F8T2) by steady state optical spectroscopy. In addition to the individual emissions of PFO and P3HT chromaphores, blends show a new peak emission around 590 nm, resulting in a full range white emission from blue to red wavelengths, 400 nm – 750 nm. The new peak is attributed to well dissolved, 'isolated', P3HT chains dispersed into the PFO matrix. It was observed that the well dissolved P3HT chains are activated by Foster energy transfer, where PFO and P3HT molecules act as donor and acceptor, respectively. Further, emission from ordered aggregates of P3HT are clearly observed and the interplay between aggregate and isolate P3HT chains was studied. In contrast to the emission results of the blends, the F8T2 co-polymer emission spectra shows a clear interaction in the ground state between the PFO and P3HT monomer-units, giving a wholly new chromaphore on the backbone.

[Poster#08]

Using Resonance Raman Scattering and Isotopic Substitution Techniques to Probe AIE Process from Theoretical Insight

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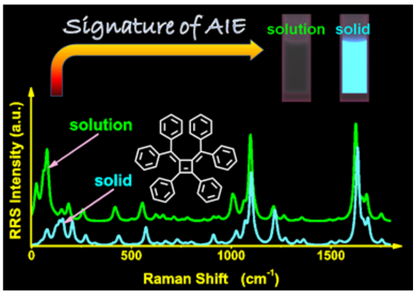
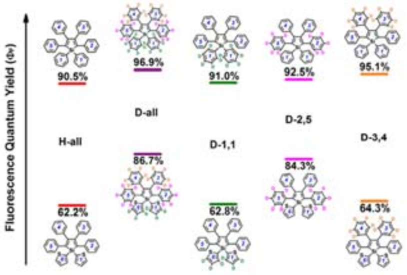
The restricted non-radiative intramolecular relaxation, which has been suggested to be crucial to the AIE process, is still hard to verify directly. We propose to use the resonance Raman scattering and isotopic substitution techniques to track the non-radiative decay process of the AIE luminogen. The restricted non-radiative relaxation pathways as a consequence of aggregation in 1,2-diphenyl-3,4-bis(diphenylmethylene)-1-cyclobutene (HPDMCb)[1], could leave a spectroscopic signature of remarkable blue-shifted and depressed low-frequency peaks on resonance Raman spectroscopy (RRS),[2] because RRS amplitude is proportional to the mode's relaxation energy during the vibronic coupled process times frequency.





We also probed different isotope effects for the AIEgen in solid crystal as compared to aqueous solution, taking examples of 1,1,2,3,4,5-hexaphenylsilole (HPS)[3] and 1,1-bis(2'-thienyl)-2,3,4,5-tetraphenylsiolole (BtTPS)[4]. We find the fully-deuterated cluster will exhibit observable enhanced luminescence comparing with the pristine cluster, while leaving the deuterated solution still dark. Furthermore, the position-dependent deuteration effects on the non-radiative decay process are predicted.

References

[1] Dong, Y. Q., Lam, J. W. Y., Qin, A. J., Sun, J. X., Liu, J. Z., Li, Z., Sun, J. Z., Sung, H. H. Y., Williams, I. D., Kwok, H. S. and Tang, B. Z., "Aggregation-Induced and Crystallization-Enhanced Emissions of 1,2-Diphenyl-3,4-bis(Diphenylmethylene)-1-Cyclobutene", *Chem. Commun.*, (2007), pp 3255-3257.

[2] Zhang, T., Ma, H. L., Niu, Y. L., Li, W. Q., Wang, D., Peng, Q., Shuai, Z. G. and Liang, W. Z., "Spectroscopic Signature of the Aggregation-Induced Emission Phenomena Caused by Restricted Nonradiative Decay: A Theoretical Proposal", *J. Phys. Chem. C*, Vol. 119, No. 9, (2015), pp 5040-5047.

[3] Zhang, T., Jiang, Y. Q., Niu, Y. L., Wang, D., Peng, Q. and Shuai, Z. G., "Aggregation Effects on the Optical Emission of 1,1,2,3,4,5-Hexaphenylsilole (HPS): A QM/MM Study", *J. Phys. Chem. A*, Vol. 118, No. 39, (2014), pp 9094-9104.

[4] Chen, J. W., Xu, B., Yang, K. X., Cao, Y., Sung, H. H. Y., Williams, I. D. and Tang, B. Z., "Photoluminescence Spectral Reliance on Aggregation Order of 1,1-Bis(2'-thienyl)-2,3,4,5-tetraph enylsilole", *J. Phys. Chem. B*, Vol. 109, No. 36, (2005), pp 17086-17093.

[Poster#09]

Tuning of Intramolecular Charge Transfer Reactions in Dipolar Pyrrolo-pyrimidine Derivatives and Their Fluorescence Sensing Properties

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Derivatives of the nitrogen heterocycle pyrrolo-pyrimidine are widely investigated due to their bio-medical activity. Their π-conjugated backbones, leading to efficient fluorescence give rise to their applications in a wide range of electronic and optoelectronic devices. The combination of these attributes could lead to potential applications of pyrrolo-pyrimidine compounds as materials for bio-sensing and bio-labelling.

Here we present the photophysical properties of novel donor-acceptor-type chromophores based on pyrrolo-pyrimidine cores. The influence of the introduction of polar hetero-aryl moieties into the backbone of π-extended systems on the photophysical properties of the new compounds was investigated. The fluorescence properties of the novel derivatives were studied in solvents of increasing polarity and unveiled a non-monotonous variation of fluorescence efficiency determined by two competing excitation deactivation mechanisms: the decrease of radiative relaxation rate due to enhanced intramolecular charge transfer and the decrease of non-radiative relaxation rate most likely induced by the enhanced intersystem crossing to triplets.

Moreover, these novel compounds were subjected to studies of the susceptibility of the fluorescence properties to a range of metal ions in various surroundings. Extreme enhancement of fluorescence intensity, up to 400 times, was found for dimethylamine substituted pyrrolo-pyrimidine derivative, manifesting pronounced selectivity to Hg ions. The mechanism of ion sensing is discussed in frames of intramolecular charge transfer tuning.

[Poster#10]

Tuning the Optical Properties of Dipolar Derivatives of 1,8-Naphthalimide: Effects of the Substituents and the Environment

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Organic electroactive molecules possessing both donor and acceptor substituents are of increasing importance for the application in optoelectronic devices such as organic light emitting diodes, bulk heterojunction solar cells and sensors. The unique structure of donor-acceptor molecules allows their optical and electrochemical properties to be tuned finely over a wide range by appropriate chemical modification of the donor and acceptor moieties. The further progress in the design and synthesis of the donor-acceptor systems depend to the great extent on understanding the structure-property relationship of such compounds. Excitation relaxation pathways in donor-acceptor systems are intricate due to intramolecular charge transfer, which is highly sensitive to the wavefunction overlap between the electron-donating and electron-accepting systems and the twisting angle of the conjugated fragments. Excitation relaxation includes charge transfer and n-π states that are highly sensitive to the twisting angle and polarity of the surrounding medium. Moreover, it includes relaxation pathway via the triplet states that attracted special attention recently due to their importance in emitters based on delayed fluorescence.

Owing to the extended π-electron system, 1,8-naphthalimide derivatives represent an attractive class of organic materials with electron-deficient moiety and showing high electron affinity. They have variable energy bandgap and often exhibit pronounced charge-transporting and fluorescence properties. Here we analyze the properties of 1,8-naphthalimide derivatives singly bonded at C-4 position by aromatic substituents, which vary in polarity and the size of their pi-conjugated system. The intramolecular twisting of the donor and acceptor moieties and the wave function overlap are assessed by DFT modeling, supplemented by experimental data on the optical properties of the compounds in various surrounding. The excitation recombination pathways were tested both for singlet ant triplet excitations including their intermediate charge-transfer states. Remarkable tuning possibilities of the emission quantum yield are demonstrated for compounds possessing steric and polar substituents. Moreover, these compounds were subjected to studies of the susceptibility of the fluorescence properties to a range of metal ions in various surroundings. Extreme sensitivity (of more than 4000 times) and selectivity to mercury ions was disclosed for naphthalimide substituted with dimethylamine.

[Poster#11]

Light-emitting Polycyclic Aromatic Hydrocarbon Synthesized by Regioselective Photocyclization and Its Application in Optical Waveguide

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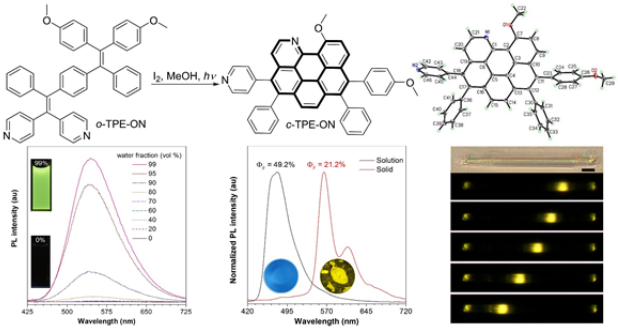
Polycyclic aromatic hydrocarbons (PAHs) are known as “pieces of graphene” and have been regarded as an important class of materials in recent years.[1,2] In particular, PAH-based luminescent materials with readily tunable electronic and optical properties have wide applications in optical waveguides, optically pumped lasers, and light-emitting diodes. However, these materials suffer the problem of aggregation-caused quenching effect (ACQ) in the solid state, which seriously limits their real-world applications. In 2001, Tang and coworkers observed a phenomenon of aggregation-induced emission (AIE) in some propeller-shaped molecules, which was exactly opposite to the ACQ effect.[3] Materials with AIE features exhibit high emission efficiency in the solid state. Because of this, it is of interest to endow PAHs with AIE properties because it may open a new pathway to construct efficient solid-state emitters for high-technological applications. In this work, a new PAH, abbreviated as *c*-TPE-ON, with an unexpected regioselectivity was obtained by controllable partial photocyclization of an AIE-active luminogen named *o*-TPE-ON. The structure of *c*-TPE-ON was confirmed by X-ray single crystal diffraction analysis, and the unexpected regioselectivity was explained by DFT calculation. Interestingly, *c*-TPE-ON with a rigid polycyclic aromatic plate displays high quantum yields both in solution (49.2%) and in the solid state (21.2%). This is due to the inhibition of emission quenching by strong π-π stacking interaction due to the steric hindrance of the unlocked twisted phenyl rings at the peripheries. The micro-rods of *c*-TPE-ON show an excellent optical waveguide property. Thus, *c*-TPE-ON is a new light-emitting PAH and is a promising material for fabricating organic optoelectronic devices.



References

[1] Havey R. G., “Polycyclic Aromatic Hydrocarbons”, Wiley-VCH, New York (1997).

[2] Figueira-Duarte T. M. and Müllen K., “Pyrene-based materials for organic electronics”, *Chem. Rev.*, Vol 111, No. 11, (2011), pp 7260-7314.

[3] Hong Y., Lam J. W. Y. and Tang B. Z., “Aggregation-induced emission”, *Chem. Soc. Rev.*, Vol 40, (2011), pp 5361-5388.

[Poster#12]

Bipolar Gold(III) Complexes for Solution-Processable Organic Light-Emitting Devices with a Small Efficiency Roll-Off

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A new class of bipolar alkynylgold(III) complexes containing triphenylamine and benzimidazole moieties has been synthesized and fully characterized. The incorporation of methyl groups in the central phenyl unit has been found to rigidify the molecule to reduce non-radiative decay, yielding a high photoluminescence quantum yield of up to 75 % in spin-coated thin films. More importantly, this class of alkynylgold(III) complexes exhibits excellent solubility in various organic solvents and is capable of serving as phosphorescent dopants in the fabrication of solution-processable organic light-emitting devices (OLEDs). Efficient solution-processable OLEDs with high external quantum efficiency (EQE) of up to 10 % and an extremely small efficiency roll-off of less than 1 % at a practical brightness of 1000 cd m^{-2} have been demonstrated.

References

[1] M.-C. Tang, D. P.-K. Tsang, Y.-C. Wong, M.-Y. Chan, K. M.-C. Wong, V. W.-W. Yam. *J. Am. Chem. Soc.*, **2014**, *136*, 17861.

[Poster#13]

Emission Mechanisms and Applications of Phenylbenzoxales Based AIE Compounds

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A series of arylbenzoxales based AIE (aggregation-induced emission)-active compounds have been synthesized via simple procedures. Small tuning of molecular structure can cause dramatic change of emission mechanism, as investigated by theoretical calculations and photophysical experiments. These mechanisms include restriction of photoinduced twisted intramolecular charge transfer, specific molecular stacking (J-aggregation,cross stacking) or a combination of both[1-4] (Figure 1), depending greatly on the subtle tuning of molecular structures. These AIE materials may find good applications such as OLED, organogel and bioimging[4-6].

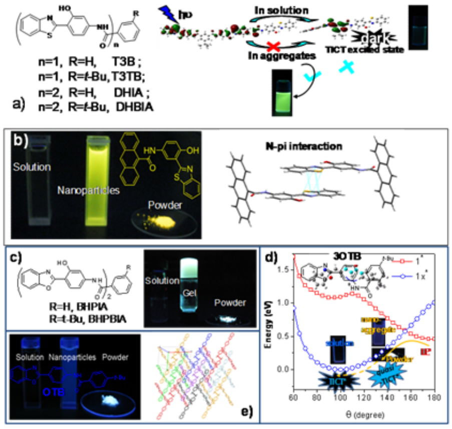

Figure 1. AIE mechanisms of arylbenzoxales based compounds

References

[1] Li, J., Qian, Y., Xie, L., Yi, Y., Li, W. and Huang, W., "From Dark TICT State to Emissive quasi-TICT State: The AIE Mechanism of N-(3-(benzo d oxazol-2-y1)phenyl)-4-tert-butylbenzamide", *Journal of Physical Chemistry C,* Vol. 119, No. 4, (2015), pp 2133-2141.

[2] Qian, Y., Cai, M., Zhou, X., Gao, Z., Wang, X., Zhao, Y., Yan, X., Wei, W., Xie, L. and Huang, W., "More than Restriction of Twisted Intramolecular Charge Transfer: Three-Dimensional Expanded #-Shaped Cross-Molecular Packing for Emission Enhancement in Aggregates", *Journal of Physical Chemistry C,* Vol. 116, No. 22, (2012), pp 12187-12195.

[3] Qian, Y., Cai, M.-M., Xie, L.-H., Yang, G.-Q., Wu, S.-K. and Huang, W., "Restriction of Photoinduced Twisted Intramolecular Charge Transfer", *Chemphyschem,* Vol. 12, No. 2, (2011), pp 397-404.

[4] Qian, Y., Li, S., Wang, Q., Sheng, X., Wu, S., Wang, S., Li, J. and Yang, G., "A nonpolymeric highly emissive ESIPT organogelator with neither dendritic structures nor long alkyl/alkoxy chains", *Soft Matter,* Vol. 8, No. 3, (2012), pp 757-764.

[5] Tu, Z., Liu, M., Qian, Y., Yang, G., Cai, M., Wang, L. and Huang, W. "Easily fixed simple small ESIPT molecule with aggregation induced emission for fast and photostable "turn-on" bioimaging ", *Rsc Advances,* Vol. 5, No. 10, (2015), pp 7789-7793.

[6] Ye, J., Liu, C., Ou, C., Cai, M., Chen, S., Wei, Q., Li, W., Qian, Y., Xie, L., Mi, B., Gao, Z. and Huang, W. "Universal Strategy for Cheap and Color-Stable Single-EML WOLEDs Utilizing Two Complementary-Color Nondoped Emitters without Energy Transfer", *Advanced Optical Materials,* Vol. 2, No. 10, (2014), pp 938-944.

[Poster#14]

Material Selection for Donor Materials in Small Molecular-Based Bulk Heterojunction Organic Photovoltaic Devices

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Organic photovoltaic (OPV) devices are considered as a promising renewable energy source due to their distinct properties over the inorganic counterparts. Extensive efforts on the development of smart materials and innovative device architecture have boosted the power conversion efficiency up to 12 %. In particular, bulk heterojunction consisting of a spatially distributed donor/acceptor interface is the most efficient approach, in which almost all excitons can be effectively dissociated into free carriers to yield 100 % exciton dissociation efficiency and generate high photocurrent. However, the major challenge for achieving high power conversion efficiency is the relative poor charge carrier mobilties in the blended layer; especially the charge carrier mobilites in the blended layer are orders of magnitude lower than those of homogeneous layers. Recent demonstration on the use of a modified bulk heterojunction opens up a new avenue for improving the performance of OPV devices, in which a non-absorbing donor material at very low dopant concentration is doped into fullerene matrix to form the bulk heterojunction. Surprisingly, the doping of non-absorbing organic materials (i.e. 5 %) can dramatically improve the photovoltaic responses including short-circuit current, open-circuit voltage (Voc), and fill factor, which is the highest ever reported for a cell with fullerene as the sole absorber. On the other hand, the exact mechanism for the performance improvement is not well-understood. The common energy gap law for Voc cannot be applied. Here, the effects of different non-absorbing organic materials as donor on the performance of OPV devices with the modified bulk heterojunction have been systematically studied and the correlation between the physical and energetic properties of donor materials and the photovoltaic responses will be discussed.

[Poster#15]

Singlet Fission in Mixed Films of Pentacene and Perfluoropentacene

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Singlet Fission (SF), the spin-allowed process by which a singlet exciton becomes two triplet excitons, has been shown to increase the efficiency of photovoltaic devices. Charge transfer (CT) states play an important role in this process. To further learn about the characteristics of CT states, we study mixed films of three different ratios of pentacene (PEN) and perfluoropentacene (PFP) on silica (SiO_2). We also compare the mixed films to films of pure PEN and pure PFP. Transient absorption measurements of these films reveal how CT states affect the dynamics of these systems, which could offer further insight into the singlet fission process.

[Poster#16]

Excited State Transitions of the Emissive Intramolecular Charge-transfer States in Thermally Activated Delayed Fluorescence Molecules

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Materials showing thermally activated delayed fluorescence (TADF) have the ability to achieve 100 % internal quantum efficiency in working devices (OLEDs) and thus are able to supersede the limitation imposed by spin statistical charge recombination. [1] This process is attainable through use of intramolecular charge-transfer (CT) states formed between the electron donor and acceptor molecules. [2] However the exact mechanisms that allow efficient emission are still unknown, particularly the role of molecule structure and the ordering of energy levels. Here we use quasi-CW pump probe measurements and time resolved flash photolysis to investigate the kinetics of reverse inter system crossing of the excited states formed in these systems. Through direct excitation of the CT states and through indirect transfer from the local excitons the significance of the energetic ordering on the recombination kinetics of TADF will be unveiled.

References

[1] H. Uoyama, K. Goushi, K. Shizu, H. Nomura, and C. Adachi, Nature **492**, 234 (2012).
[2] V. Jankus, P. Data, D. Graves, C. McGuinness, J. Santos, M. R. Bryce, F. B. Dias, and A. P. Monkman, Adv. Funct. Mater. n/a (2014).

[Poster#17]

The Influences of Host Matrix and D-A Molecular Geometry on Thermal Assisted Delayed Fluorescence and Device Performance

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Thermal assisted delayed fluorescence (TADF) has been investigated as a way to improve the performance of organic light diodes (OLEDs), due to the possibility of harvesting 'dark' triplet excited states. The TADF mechanism requires the up-conversion of triplets into more energetic but emissive singlet states. The efficiency of this mechanism is controlled by two main parameters, the energy splitting between the singlet and triplet states (ΔE_{ST}), which needs to be minimized, and the presence of non-radiative pathways available for the excited singlet and triplet states to decay. These need to be suppressed in order to obtain high fluorescence quantum yields and long triplet excited state lifetimes.
Molecules formed by strong electron donor (D) and electron acceptor (A) units, which form stable charge transfer excited states, are the best candidates to show efficient TADF, due to their small singlet-triplet energy gap. In order to suppress triplet-triplet annihilation (TTA), which is often operative in thin films and rapidly quenches the triplet population, small TADF molecules are dispersed in host matrixes with high triplet energy levels.[1]

Unfortunately, host-guest and guest-guest interactions often influence the photoluminescent (PL) and electroluminescent (EL) properties of TADF emitters, causing large variations on the emission yield and lifetime due to the formation of exciplexes that may work as energy traps. The TADF mechanism is in general well understood, the role of molecular geometry and molecular interactions on the TADF efficiency is still unclear.[2,3]

Here, we report the study of a family of D-A molecules based on a phenothiazine donor (D) and a dibenzothiophene-S,S-dioxide acceptor (A), covalently linked in near perpendicular D-A orientation, as confirmed by single-crystal X-ray data. The excited state dynamics of these molecules is strongly affected by the surronding medium, showing fast population of charge transfer singlet and triplet states. Time resolved fluorescence measurements were performed in solution of different solvents, and solid thin films with different hosts to evaluate the effect of TADF on device performance.

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References

[1] F. B. Dias, K. N. Bourdakos, V. Jankus, K. C. Moss, K. T. Kamtekar, V. Bhalla, J. Santos, M. R. Bryce, A. P. Monkman, *Adv. Mater.* **2013**, 25, 3707.
[2] G. Méhes, K. Goushi, W. J. Potscavage, Jr., C. Adachi, *Organic Electronics* **2014**, 15 2027.
[3] V. Jankus, P. Data, D. Graves, C. McGuinness, J. Santos, M. R. Bryce, F. B. Dias, A. P. Monkman, *Adv. Funct. Mater.* **2014**, 24, 6178.

[Poster#18]

Development of Pure Organic Materials with Long-Lived and Efficient Room Temperature Phosphorescence

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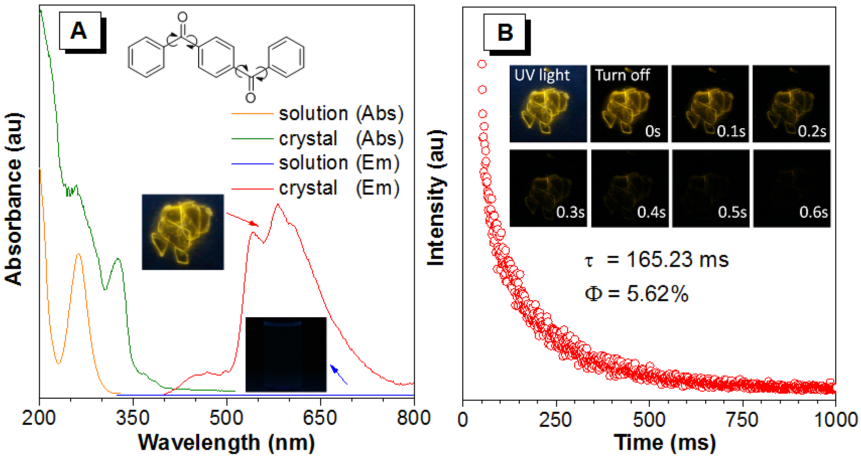
The phosphorescent emission of pure organic materials is known to be ineffective at room temperature, which thus makes them fail to enter discussions on modern phosphorescent applications.[1] However, the development of phosphors is a goal of intensive research for their potential applications in organic electronics and chemical and biological detection.[2 4] In this work, 1,4-phenylenebis(phenylmethanone) (DPB) and its derivatives are prepared and their optical properties are investigated. DPB and its derivatives are not emissive in either solution or amorphous state. They, however, emit strong phosphorescence in the crystal state. Their luminescence lifetimes are measured to be more than 0.1s, which is quite long among the room-temperature organic phosphors reported so far.[3] By incorporation of appropriate substituents, phosphors with multiple emission colors are obtained. Among all the substituted DBPs, the chlorine-containing one exhibits the highest phosphorescent quantum yield of 32.2%.



References

[1] Kohler A., Wilson JS. and Friend RH., “Fluorescence and Phosphorescence in Organic Materials”, *Adv. Mater.*, 14, (2002), 701–707.

[2] Baldo MA., O'Brien DF., You Y., Shoustikov A., Sibley S., Thompson ME. and Forrest SR., “Highly efficient phosphorescent emission from organic electroluminescent devices”, *Nature* 395 (1998), 151–154.

[3] Rumsey WL., Vanderkooi JM. and Wilson DF., “Imaging of phosphorescence: a novel method for measuring oxygen distribution in perfused tissue”, *Science* 241 (1998), 1649–1651.

[4] Zhang G., Palmer GM., Dewhirts MW. and Fraser CL., “A dual-emissive-materials design concept enables tumour hypoxia imaging”, *Nature Mater.*, 8, (2009), 747–751.

[Poster#19]

High Efficiency Green Phosphorescent Organic Light-emitting Diode Based on Simplified Device Structures

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A high efficiency green phosphorescent organic light emitting diode with simplified structure was achieved free of hole transport layer. The design of this kind of device structure not only saves the consumption of organic materials but also greatly reduces the structural heterogeneities and effectively facilitates the charge injection into the emissive layer. The resulting green PHOLEDs exhibit higher electroluminescent efficiency. The maximum external quantum efficiency and current efficiency reach 23.7% and 88 CdA^{-1}, respectively. Moreover the devices demonstrate satisfactory stability, keeping 23.7% and 88 CdA^{-1}, 22 and 82 CdA^{-1}, respectively, at a luminance of 100 and 1000 Cdm^{-2}. The working mechanism for achieving high efficiency based on such simple device structure is discussed correspondingly. The improved charge carrier injection and transport balance were proved to prominently attribute to achieve the high efficiency and great stability at high luminance in the green PHOLEDs.

References

[1]J. Kido, M. Kimura, K. Nagai, “Multilayer White Light-Emitting Organic Electroluminescent Device”, *Science,* vol. 267(1995) 1332-1334.

[2]Z. Shen, P. E. Burrows, V. Bulovic, S. R. Forrest, M. E. Thompson, “Three-Color, Tunable, Organic Light-Emitting Devices”, *Science*, vol. 276(1997) 2009-2011.

[3]O. Fadhel, M. Gras, N. Lemaitre, V. Deborde, M. Hissler,B. Geffroy, and R. Réau, “Tunable Organophosphorus Dopants for Bright White Organic Light-Emitting Diodes with Simple Structures”, *Adv. Mater*., vol. 21(2009) 1261-1265.

[4]W. S. Jeon, T.J. Park, S.Y. Kim, R. Pode, J. Jang, J.H. Kwon, “Low roll-off efficiency green phosphorescent organic light-emitting devices with simple double emissive layer structure”, *Appl. Phys.Lett*., 93 (2008)063303.

[5]J. Meyer, S. Hamwi, T. Bülow, H.-H. Johannes, T. Riedl, W. Kowalsky,“Highly efficient simplified organic light emitting diodes”,*Appl. Phys. Lett.*, 91 (2007),113506

[Poster#20]

Construction of Efficient Deep Blue AIE Luminogen from Triphenylethene for Non-Doped OLED Applications

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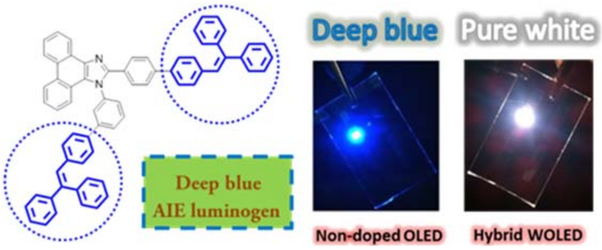

Chart 1. Chemical structure of BTPE-PI for non-

Deep blue emitters are crucial for full color displays and organic white lighting. Thanks to the research efforts by scientists, many efficient light emitters with aggregation-induced emission (AIE) characteristics have been synthesized and found promising applications in organic light-emitting devices (OLEDs).[1,2] However, few AIE emitters with deep blue emission and excellent electroluminescence (EL) performance have been reported. In this work, we report a simple but successful molecular design strategy for fabricating efficient non-doped OLEDs with both deep blue and white emission. This strategy utilizes triphenylethylene,[3] a weak conjugated AIE luminogen, as a building block for emitter construction, thus involving no control on the light emission process through adjustment of the steric hindrance of chromophores and allowing a wide selection of partnered functional units. The synthesized AIE luminogen, abbreviated as BTPE-PI, is thermally stable and exhibits high fluorescence quantum efficiency as well as balanced charge injection capability in the solid state (Chart 1). Non-doped deep blue OLED fabricated from BTPE-PI shows high external quantum efficiency of 4.4% with a small roll-off, which is among the best EL performance for deep blue AIE materials. An efficient hybrid white OLED with Commission Internationale de l'Eclairage (CIE) coordinates of (0.33, 0.33) at theoretical white point was first achieved by BTPE-PI as deep blue emitter. Such novel molecular design strategy opens a new avenue in the development of efficient solid-state deep blue emitters for non-doped OLED applications.

References

[1] Hong Y., Lam JWY. and Tang BZ., "Aggregation-Induced Emission: Phenomenon, Mechanism and Applications", *Chem. Commun.* (2009), 4332–4353.
[2] Mei J., Hong Y., Lam JWY., Qin A., Tang Y. and Tang BZ., "Aggregation-Induced Emission: The Whole Is More Brilliant than the Parts", *Adv. Mater.*, 26, (2014), 5429–5479
[3] Yang Z., Chi Z., Yu T., Zhang X., Chen M., Xu B., Liu S., Zhang Y. and Xu, J. "Triphenylethylene Carbazole Derivatives as a New Class of AIE Materials with Strong Blue Light Emission and High Glass Transition Temperature", *J. Mater. Chem.*, 19, (2009), 5541–5546.

[Poster#21]

Realization of Ultra-high Color Stable Hybrid White Organic Light-emitting Diodes via Sequential Symmetrical Doping in Emissive Layer

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White organic light emitting diodes (WOLEDs) have attracted considerable attentions in the past two decades due to their advantages of energy saving, large area, thin and flexibility for application in full-color flat-panel displays and solid state lighting. To produce high efficiency WOLEDs, hybrid WOLEDs that incorporate high performance fluorescent blue emitters with appropriate phosphorescent dopants emitting at long wavelength regions have been proposed. In typical hybrid WOLEDs, fluorescent blue materials are often doped in a host material because of the concentration quenching effect of blue fluorescent emitters, making a rather complicated control in device fabrication while other phosphorescent emitters are also doped into the same host. When the fabrication of hybrid WOLEDs involves the simultaneous doping of fluorescent blue emitter, phosphorescent yellow and red dopants in the same host, the color quality of the hybrid WOLEDs must be controlled accurately by adjusting the doping concentrations of different emitters, which is not favorable process for eventual efficient mass production.

In this work, high performance three-color hybrid WOLED has been demonstrated by emissions from a fluorescent blue emitter 5,11-di(40-dimesitylboronphenyl) indolo[3,2-b]carbazole (DDBICZ), a phosphorescent yellow emitter bis(2-(3-trifluoromethyl-4-fluorophenyl)-4-methylquinolyl)(acetylacetonate)iridium(III) ($Ir(ffpmq)_2(acac)$) and a phosphorescent red emitter bis(1-phenylisoquinoline) (acetylacetonate)iridium(III) ($Ir(piq)_2(acac)$). From the device, the blue emitting DDBICZ also acts as a trip host for $Ir(ffpmq)_2(acac)$ and $Ir(piq)_2(acac)$ dopants. The emissive layer in the DDBICZ-based hybrid WOLEDs consists of a sequential symmetric doping configuration for achieving high color stability, CIE color coordinates of (0.40, 0.41) and color rendering index of 86 over the brightness range from 10 cd/m^2 to 10,000 cd/m^2.

[Poster#22]

Improved Electron Injection Efficiency in Organic Light-emitting Diodes Using p/n Heterojunction Injection Contact

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Efficient charge injection is a prerequisite for achieving low turn-on voltage and improved hole-electron current balance in OLEDs. Charge injection layer, p-doped or n-doped organic interlayer is commonly used for reducing the energy barrier at the organic/metal interface for efficient charge injection. In this work, a pentacene/C_{60}-based bilayer p/n heterojunction is interposed at the interface between the cathode and the organic to improve the electron injection in OLEDs. The effect of p/n junction on charge injection was analyzed and varied using OLEDs having a fluorescent EL unit (organic stack: CFx/NPB/Alq_3) and a phosphorescent EL unit (organic stack: CFx/TAPC/CBP:Ir(ppy)2acac/TmPyPB), e.g., OLEDs with a configuration of ITO/organic stack/ LiF(1 nm)/Al(1.5 nm)/p-n heterojunction/Al(100 nm). It is shown that p/n heterojunction-modified cathode allows improving electron current and thereby efficiency of OLEDs. The results also reveal that the interposing a bi-layer p/n heterojunction between the cathode and the functional organic stack making the electron injection that is less dependent on the choice of the cathode materials.

[Poster#23]

Inverted OLED Integrated with Oxide Thin Film Transistor Using Hybrid Structure

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Oxide thin film transistors (TFTs) are considered as the main backplane technology for future's OLED TV since its high electron mobility, good large area uniformity and low power consumption. However, most oxide TFTs have the n-type feature. Thus, inverted structure is preferred for OLEDs compared to the conventional structure for the sake of simpler driving circuit design. In this work, hybrid inverted OLED was fabricated with inorganic electron transportation layer (ETL), like ZnO or IGZO. Because there exist a large energy difference between the LUMO of emitting material and the conduction band of ETL. A thin polymer polyethylenimine ethoxylated (PEIE) [1] layer was used as electron injection layer (EIL) to overcome the large electron barrier, as shown in Figure 1. With this inverted structure, the ETL of OLED can be integrated onto TFT and be formed during the TFT fabrication process. Thus, mask for patterning the contact electrode can be eliminated. The performance of the inverted OLED is comparable with that of its counterpart.

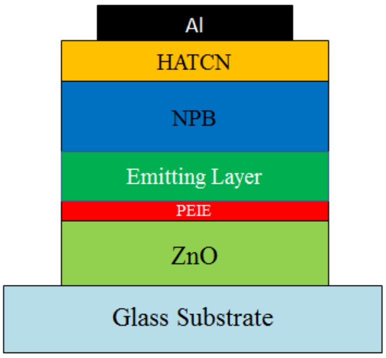

Figure 1. Layer structure of inverted OLED

References

[1] Y.H. Zhou, C. Fuentes-Hernandez, J.W. Shim, J. Meyer, A. Giordano, H. Li, P. Winget, T. Papadopoulos, H.S. Cheun, J.B. Kim, M. Fenoll, A. Dindar, W. Haske, E. Najafabadi, T. Khan, H. Sojoudi, S. Barlow, S. Graham, J.L. Brédas, S. Marder, A. Kahn, B.A. Kippelen, "Universal method to produce low-work function electrodes for organic electronics", *Science* 336 (2012) 327.

[Poster#24]

A Dual-Functional AEE Fluorogen as A Mitochondrion-Specific Bioprobe and an Effective Photosensitizer for Photodynamic Therapy

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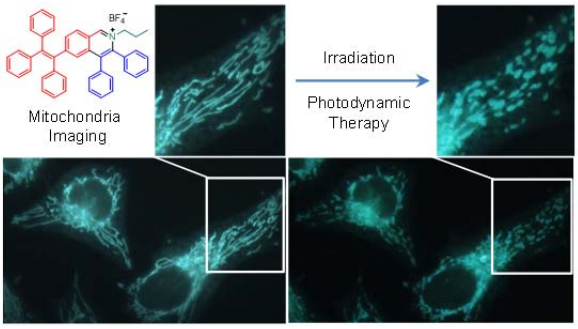
Photodynamic therapy (PDT) has gained increasing attention due to its higher selectivity and less side effect than chemotherapy in cancer elimination.[1,2] Mitochondria are the powerhouse of cell and the key organelle regulating the cell apoptosis process. Targeting mitochondria will undoubtedly increase the effectiveness in PDT.[3] In this work, we report a dual-functional luminogen with aggregation-enhanced emission feature abbreviated as TPE-IQ. This luminogen can target and light up mitochondria in both live and fixed cells with superb selectivity and high signal-to-noise ratio. More intriguingly, TPE-IQ can serve as a photosensitizer, generating reactive oxygen species to induce cell apoptosis upon photoexcitation. The high selectivity towards mitochondria makes TPE-IQ an effective and efficient sensitizer for PDT, while the imaging functionality of TPE-IQ facilitates the monitoring of the morphological change of mitochondria and tracking the position of the cancer cells simultaneously.



Scheme 1. Illustration of the mitochondria-imagingand

References

[1] Celli JP., Spring BQ., Rizvi I., Evans CL., Samkoe KS., Verma S., Pogue BW. and Hasan T., “Imaging and Photodynamic Therapy: Mechanisms, Monitoring and Optimization”, *Chem. Rev.,* 110 (2010), 2795–2838.
[2] Ethirajan M., Chen Y., Joshi P. and Pandey RK., “The role of porphyrin chemistry in tumor imaging and photodynamic therapy”, *Chem. Soc. Rev.,* 40 (2011), 340–362.
[3] Modica-Napolitano JS. and Aprille JR., “Delocalized lipophilic cations selectively target the mitochondria of carcinoma cells”, *Adv. Drug Deliv. Rev.,* 49 (2001), 63–70.

[Poster#25]

An AIE-Active Turn-On Bioprobe Mediated by Hydrogen Bonding for Highly Sensitive Detection of Hydrogen Peroxide and Glucose

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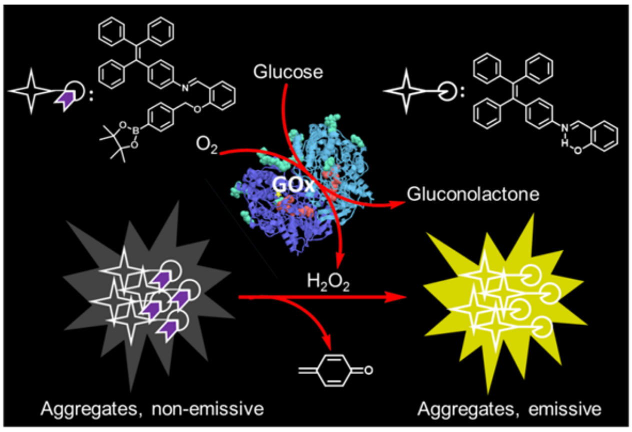
Hydrogen peroxide detection is of great significance for environment monitoring and metabolism of living organisms.[1] Imine group serves as an efficient fluorescent quencher but the quenching effect is impaired when the electron lone pair of the nitrogen atom forms hydrogen bond with adjacent protons. Therefore, such hydrogen bonding serves as a mechanism for hydrogen peroxide detection by most imine-functionalized fluorophores.[2] Herein, an AIE-active "turn-on" bioprobe for hydrogen peroxide detection is designed rationally based on a tetraphenylethene-containing Schiff base. The probe is non-emissive in buffer solutions but when treated with hydrogen peroxide, bright yellow fluorescence is observed due to the formation of intramolecular hydrogen bond in the hydrolyzed product. The linear fluorescence response enables quantification of hydrogen peroxide in the range of 0–100 μM with superior sensitivity and selectivity. Since hydrogen peroxide is generated enzymatically through glucose oxidation process catalyzed by glucose oxidase, assay of glucose is successfully achieved in buffer solutions and serum samples, showing the potential application in diagnosis of diabetes (Scheme 1).[3]



Scheme 1. Schematic illustration of hydrogen

References

[1] Giorgio M., Trinei M., Migliaccio E. and Pelicci PG., "Hydrogen peroxide: a metabolic by-product or a common mediator of ageing signals?", *Nat. Rev. Mol. Cell Biol.*, 8, (2007), 722–728.
[2] Wu J., Liu W., Ge J., Zhang H. and Wang P., "New sensing mechanisms for design of fluorescent chemosensors emerging in recent years, *Chem. Soc. Rev.*, 40, (2011), 3483–3495.
[3] Mei J., Hong Y., Lam JWY., Qin A., Tang Y. and Tang BZ., "Aggregation-Induced Emission: The Whole Is More Brilliant than the Parts", *Adv. Mater*., 26, (2014), 5429–5479

[Poster#26]

A Photostable AIE Fluorogen for Nucleolus and Mitochondrion Imaging with Organelle-specific Emission

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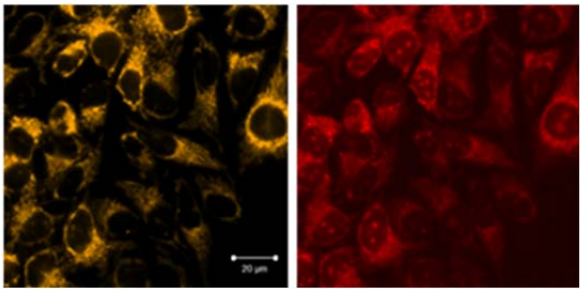

Figure 1. Confocal images of HeLa cell stained with ASCP. Ex.: (left) 405 nm and (right) 560 nm.

The nucleolus is the key site in the nucleus for the synthesis and assembles of ribosomal RNAs (rRNA). Its functions are tightly related to cell growth and proliferation.[1] It is known that the nucleolar rRNAs assemble during the late telophase and throughout the interphase, but dissemble when the cells undergo mitosis.[2] However, details about the nucleolar dynamic mechanisms of intracellular distribution, trafficking, and localization throughout a complete cell cycle are still under investigation. In pre-fixed cells, it is difficult to study the nucleolar dynamic. A fluorescent nucleolus-selective probe can help to observe the nucleolus-related events. Up to date, there is only one commercially available dye called SYTORNASelect for RNA imaging in live cell. However, in term of selectivity and photostability, its performance is not good. On the other hand, mitochondria play an important role in life and death of cells and are related to several human diseases. Tracking the morphological change of mitochondria can help study the apoptosis and degenerative process. Doing so, a photostable mitochondrion-selective dye is required. However, most of the commercially available mitochondrion-selective dyes show weak photostabilty. In this work, we prepared a dual targeting fluorogen, abbreviated as ASCP, for mitochondria and nucleolus imaging. It shows orange color in mitochondria and red color in nucleolus and enjoys good photostability (Figure 1).

References

[1] Yusupov M. M., Yusupova G. Z., Baucom A., Lieberman K., Earnest T. N., Cate J. H. D. and Noller H. F., “Crystal structure of the ribosome at 5.5 Å resolution.” *Science*, Vol 292, No. 5518, (2001), pp 883-896.

[2] Hernandez-Verdun D., Roussel P. and Gébrane-Younès J., “Emerging concepts of nucleolar assembly.” *J. Cell Sci.*, Vol 115, No. 11, (2002), pp 2265-2270.

[Poster#27]

Plasmonic-Electrical Effect on Organic Solar Cell by the Incorporation of Metallic Nanostructures

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Recently, plasmonic effects of metal nanostructures have been intensively exploited to enhance the performance of organic solar cells (OSCs). The plasmonic-optical effects of localized surface plasmon resonances (LSRPs), scattering effect and propagating surface plasmon resonances (SPRs) etc. are well recognized in considerably enhancing performance of OSCs [1]. Through embedding metallic nanostructures into active layer, carrier transport layer (CTL) or introducing the nanopatterned electrode, the plasmonic-optical effects of metallic nanostructures can contribute to enhance the active layer absorption. Moreover, the enhancement of active layer absorption can be further improved and broadened through incorporating metal nanostructures with different shapes (nanospheres, nanoprisms, naonrods), different materials (silver, gold, copper, aluminum etc.), multiple structures into active layer and CTL and engineering metal nanopatterned electrode into quasi-periodic structures and wrinkle surface.[2]

However, the overall device efficiency is not only limited by the optical absorption of active layer but also next constrained by the electrical properties of OSCs such as locations of exciton generation, mobility of charge carriers, interfacial morphologies and extraction of charge carriers etc. In recent, the incorporation of metal structures has been reported to improve these electrical properties of OSCs.[3] For instance, the mobility of the charge carriers in organic materials incorporated by the embedded metal NPs was enhanced with two folds and also the better interfacial morphology between organic and CTL has been demonstrated to favor the charge carrier extraction. Besides, the plasmonic of metal nanostructures induced space-charge limit (SCL) elimination, transfer of plasmonically excited hot carriers and charge-accumulation effects that termed by plasmonic-electrical effects were recently reported to improve performance of OSCs. Therefore, the improved electrical properties of OSCs by plasmonic-electrical effects could be of equal importance in enhancing the performance of OSCs through the introduction of plasmonic metal nanostructures into different layers of OSCs.

Here, the plasmonic-electrical effects including the plasmonically excited hot carriers transfer from metal structures to metal oxide, the reduced carrier extraction barrier improved by incorporating the metal nanomaterials into CTL and the tailored exciton generation by introduction of metallic nanomaterials into active layer are discussed. The promoted electrical properties of OSCs by the plasmonic-electrical effects and the future combination of plasmonic-optical and electrical effects would promisingly offer an alternative way to further improve the performance of OSCs.

References

[1] Atwater H. A. and Polman A., "Plasmonics for improved photovoltaic devices," Nat. Mater., vol. 9, (2010), pp. 205-213.

[2] Choy W. C. H., Chan W. K., and Yuan Y. P., "Recent Advances in Transition Metal Complexes and Light-Management Engineering in Organic Optoelectronic Devices," Adv. Mater., vol. 26, (2014), pp. 5368-5399.

[3] Choy W. C.H. and Ren X.G. “Plasmonic-Electrical Effect on Organic Solar Cell by the Incorporation of Metallic Nanostructures”, IEEE, J. Sel. Top. Quantum Electron. under review.

[Poster#28]

Plasmonic-Electrical Effects in Metal Oxide Transport Layers for High-Performance Organic Photovoltaics

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Carrier transport layers are crucial to the performance of various organic optoelectronic devices. Transition metal oxides have newly emerged as promising candidates for fulfilling the role of efficient carrier transport layers due to their wide energy-aligning capabilities and stability. However, for commonly used n-type metal oxides such as TiO_2 and ZnO, light soaking is an inherent issue which prevents the device from efficiently extracting carriers when operating at long wavelength illumination outside UV region (corresponding to their bandgap).

Herein, we demonstrated and studied the charge extraction enhancement in TiO_2-based electron transport layer through utilizing metal nanoparticles (NPs) induced plasmonic-electrical effects into the metal oxide transport layer in organic solar cells (OSCs) [1]. By embedding metal (Au or Ag) NPs into solution processed TiO_2 to form the NP-TiO_2 composite as electron transport layer, the power conversion efficiencies (PCEs) of OSCs with different polymer active layers were enhanced significantly, with PCE of 8.20% and 8.74% reached in single-junction PBCTTT-C-T:PC_{71}BM- and PTB7:PC_{71}BM-based OSCs, respectively [1][2]. Furthermore, we showed that OSCs with NP-TiO_2 transport layer can operate efficiently by plasmonic light activation (at visible wavelength), in contrast to pristine TiO_2 device which can only be activated by UV light (< 400 nm). Through experimental and theorectical studies, we attributed the enhanced charge extraction in NP-TiO_2 transport layer to the distinctive plasmonic-electrical effects, through which plasmonically generated hot carriers can fill the trap states in TiO_2 and lower the effective extraction barrier under light energy far below the bandgap of pristine TiO_2 in UV region. Our work offers new routes for plasmonically enhancing the performance of various organic optoelectronic devices such as organic light emitting diodes and organic photovoltaics.

References

[1] Zhang, D.; Choy, W. C. H.; Xie, F.; Sha, W. E. I.; Li, X.; Ding, B.; Zhang, K.; Huang, F.; Cao, Y., "Plasmonic Electrically Functionalized TiO_2 for High-Performance Organic Solar Cells", *Adv. Funct. Mater.* Vol. 23, (2013), pp 4255-4261.

[2] Xie, F.; Choy, W. C. H.; Sha, W. E. I.; Zhang, D.; Zhang, S. Q.; Li, X. C.; Leung, C. W.; Hou, J. H., "Enhanced charge extraction in organic solar cells through electron accumulation effects induced by metal nanoparticles", *Energ. Environ. Sci.* Vol. 6, (2013), pp 3372-3379.

[Poster#29]

Morphology Enhancement in $CH_3NH_3PbI_3$ Perovskite Films through Vacuum-Assisted Thermal Annealing

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Recently, methylammonium lead halide perovskites ($CH_3NH_3PbI_3$) have emerged as promising materials for various optoelectronic devices with unique optical and electrical properties. In spite of the rapid advancement in perovskite research, enhancing the morphology of solution-processed perovskite films with precise control (minimizing pore formation, improving reproducibility, etc.) remains a challenging issue, while the understanding of the film formation process is not yet clear.

Here, we demonstrated that vacuum-assisted thermal annealing can be used as an effective approach to control the composition, morphology, and thus the quality of the perovskite films formed from the precursors of $PbCl_2$ and CH_3NH_3I. The critical role of the chlorine byproduct of CH_3NH_3Cl during the film formation of the perovskite was identified and investigated. Using our vacuum-assisted thermal annealing approach to completely remove the chlorine byproduct, pure, pore-free planar $CH_3NH_3PbI_3$ films with enhanced morphology can be readily formed, which exhibited high power conversion efficiency (PCE) of 14.5% in perovskite solar cells. Remarkably, the complete elimination of CH_3NH_3Cl not only considerably improves the stability and reproducibility of the perovskite device (standard deviation in PCE of only 0.92% was achieved for 60 solar cells), but also effectively suppresses photocurrent hysteresis observed in many reports of perovskite device. Consequently, our approach of vacuum-assisted thermal annealing for forming high-quality perovskite films with excellent morphology and reproducibility can lead to further performance enhancement for the various emerging perovskite optoelectronic devices.

References

[1] Xie F. X. , Zhang D., Su H, Ren X, Wong K. S., Grätzel M. and Choy W. C. H., "Vacuum-assisted thermal annealing of $CH_3NH_3PbI_3$ for highly stable and efficient perovskite solar cells" ACS Nano 9 (2015), 639.

[Poster#30]

Hole-Transporting Spirothioxanthene Derivatives as Donor Materials for Efficient Small-Molecule-Based Organic Photovoltaic Devices

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Taking the advantages of the 3D structure and rigid spiro-conjugation, spirobifluorene and its derivatives are a benchmark class of p-type semiconductors in organic electronic devices because of their good charge-transporting properties. However, their low absorption coefficients within the visible spectrum render their application as photoactive materials in the fabrication of organic photovoltaic (OPV) devices. A new class of heterocyclic spirothioxanthene derivatives has been designed and synthesized by the functionalization of the spiro core with various triarylamine groups and the modification of the heteroatom of the spiro core. The photophysical, electrochemical and thermal properties of these spirothioxanthene derivatives have been fully characterized. Of particular interest, all of these compounds exhibit high hole mobilities of up to 10–3 cm2V–1s–1, as determined from thin film transistor measurement. More importantly, these spirothioxanthene derivatives are promising donor materials for the fabrication of high performance OPV devices. With a very low dopant concentration of 7 % doped into fullerene matrix, efficient small molecular-based OPV devices with high open-circuit voltage of 0.94 V and high power conversion efficiency of 5.40 % (the highest PCE of 5.46 %) have been realized. This demonstrates for the first time their application studies as photovoltaic donor materials in OPV devices.

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References

[1] Chan C.-Y., Wong Y.-C., Chan M.-Y., Cheung S.-H., So S.-K., Yam V. W.-W., *Chem. Mater*. **2014**, *26*, 6585.

[Poster#31]

High-efficiency Non-fullerene Organic Solar Cells Enabled by a Difluorobenzothiadiazole-based Donor Polymer Combined with a Properly Matched Small Molecule Acceptor

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Here we report high-performance small molecule acceptor (SMA)-based organic solar cells (OSCs) enabled by the combination of a difluorobenzothiadiazole donor polymer named PffBT4T-2DT and a SMA named SF-PDI$_2$. It is found that SF-PDI$_2$ matches particularly well with PffBT4T-2DT and non-fullerene OSCs with an impressive V_{OC} of 0.98 V, and a high power conversion efficiency of 6.3% is achieved. Our study shows that PffBT4T-2DT is a promising donor material for SMA-based OSCs, and the selection of a matching SMA is also important to achieve the best OSC performance.

References

[1] J. Zhao, Y. Li, H. Lin, Y. Liu, K. Jiang, C. Mu, T. Ma, J. Lai, H. Hu, D. Yu and H. Yan, "High-efficiency non-fullerene organic solar cells enabled by a difluorobenzothiadiazole-based donor polymer combined with a properly matched small molecule acceptor", *Energy & Environmental Science*, Vol. 8, (2015), pp 820.

[Poster#32]

Low Threshold Lasing and Optical Properties of Vacuum-Assisted Thermal Annealed Perovskite Thin Films

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Methylammonium lead halide perovskites ($CH_3NH_3PbI_3$) have recently been identified as promising absorber materials for photovoltaic devices, combining high power conversion efficiency and low-cost production. Besides photovoltaic applications, perovskite materials possess considerable potential for many other optoelectronic devices due to the unique optical and electrical properties. Comprehensive investigation on the optical properties of the perovskite materials is highly relevant and essential to the design and development of perovskite optoelectronic devices such as lasers and light emitting device. However, the quality of the perovskite materials is predominantly affected by the processing approach, which may interfere with the accurate determination of the optical properties.

Herein, using a vacuum-assisted thermal annealing approach [1], we were able to investigate the optical properties of high-quality, pore-free and highly reproducible perovskite films by characterizing photoluminescence (PL), carrier diffusion length, defect density, etc. Electron diffusion length exceed hundreds of nanometers was observed which is comparable to recent reports [2]. We also studied the optical pumped lasing properties of our perovskite film. Amplified spontaneous emission (ASE) threshold as low as $45\mu J/cm^2$ and a gain of $369cm^{-1}$ at $127\mu J/cm^2$ pumping fluence using picosecond laser excitation was demonstrated. These ASE threshold excitation intensity and gain are as good as those report recently using femtosecond laser pumping [2], indicating high quality of our film fabricated by our unique vacuum-assisted thermal annealing method. Incorporation of distributed feedback (DFB) structure in the perovskite film further reduced the ASE threshold. More details of this work will be presented in the conference.

References

[1] Xie F. X. , Zhang D., Su H, Ren X, Wong K. S., Grätzel M. and Choy W. C. H., "Vacuum-assisted thermal annealing of $CH_3NH_3PbI_3$ for highly stable and efficient perovskite solar cells" ACS Nano 9 (2015), 639 .

[2] Stranks S. D., Eperon G. E., Grancini G., Menelaou C., Alcocer M. J. P., Leijtens T., Herz L. M., Petrozza A., Snaith H. J., "Electron-hole diffusion lengths exceeding 1 micrometer in an organometal trihalide perovskite absorber", Science 342 (2013) 241; Xing G., Mathews N., Sun S., Lim S. S., Lam Y. M., Grätzel M., Mhaisalkar S. and Sum T. C., "Long-range balanced electron- and hole-transport lengths in organic-inorganic $CH_3NH_3PbI_3$" Science 342 (2013) 244.

[3] Xing G., Mathews N., Lim S. S., Yantara N., Liu X., Dharani S., Grätzel M., Mhaisalkar S. and Sum T. C., "Low temperature solution-processed wide-wavelength-tunable perovskite for lasing" Nature Materials 13 (2014), 1.

[Poster#33]

Photophysical Characterization of Red Emitters for Solution-Processed Small-Molecule OLEDs and Organic Photovoltaic Devices

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Solution processing methods as spin-coating, spray-on and ink-jet printing allow rapid deposition over large areas at room temperature, and using flexible substrates in OLEDs and OPV devices. However, most molecules forming good films from solution, as conjugated polymers, are difficult to purify and often suffer from the presence of impurities and other defects, which rapidly quench the excited states. Multilayer deposition, as hole/electron transport and blocking layers, are also difficult to achieve in solution processed devices, due to the need of using orthogonal solvents, and avoid dissolving previous layers. This is highly detrimental to the performances of solution processed devices relative to their evaporated, but more expensive, counterparts.

In this work we discuss the photophysical characterization of four small molecule organic emitters for solution processed devices [1-2]. These are well defined small-molecule materials, with 3-5 molecular units, which allow using better purification methods and show good solubility in most organic solvents. All these molecules show extended absorption and emission in the red region, and are thus able to be used simultaneously in OLEDs and OPV devices.

This work elucidates the complex and rich photophysics of these materials and in particular addresses the role in device performances of long-lived excited states giving intramolecular thermal-assisted delayed fluorescence (E-type DF), and triplet fusion delayed fluorescence (P-type DF). The impact of molecular structure and energy ordering of electronic states is discussed on view of the application of these materials in OLED and OPV devices, giving clear guidelines for the design of new emitters.

References

[1] Huang J., Zhu X.-H., Li C., Xia Y.-J., Peng J. B., Cao Y., “Amorphous Fluorescent Organic Emitters for Efficient Solution-Processed Pure Red Electroluminescence: Synthesis, Purification, Morphology, Solid-State Photoluminescence, and Device Characterizations”, *J. Org. Chem.* Vol. *72*, (2007), pp 8580.

[2] Huang J., Liu Q., Zou J.-H., Zhu X.-H., Li A.-Y., Li J.-W., Wu S., Peng J. B., Cao Y., Xia R.-D., Bradley D. D. C., Roncali J., “Electroluminescence and Laser Emission of Soluble Pure Red Fluorescent Molecular Glasses Based on Dithienylbenzothiadiazole”, *Adv. Funct. Mater*, Vol. 19, (2009), pp 2978.

[Poster#34]

Theoretical Investigation on the Charge Transport in High-mobility Organic Semiconductors

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Up to now, an increasing number of organic field effect transistors (OFETs) based on single crystals with high mobility comes out, and the band theory, which was created for describing inorganic semiconductors (ISCs), has been used to explain such "high" mobility in organic semiconductors (OSCs). Besides, band-like temperature-dependent mobility has been observed in several organic crystals, like pentacene [1] and so on. However, none of those OSCs conforms with that electronic coupling (V) > reorganization energy (λ). Moreover, their mobilities are still far lower than those existed in ISCs, since molecules in OSCs are only bound weakly by van der Walls interactions while inorganic atoms in ISCs are covalently bonded. Thus, the scattering from intramolecular vibrations and lattice vibrations in OSCs can restrict carrier movement. Consequently, the delocalized band model may not be proper for describing charge transport in OSCs, and nuclear vibrations should be considered.

Here, we apply three methods including intramolecular electron-phonon couplings to investigate the charge transport property in those high-mobility organic semiconductors, namely, Marcus hopping theory, nuclear tunneling assisted hopping (NTAH) model, as well as time-dependent wavepacket diffusion (TDWPD) method. According to previous researches, the nuclear tunneling effect considered in the latter two approaches has been found important in charge transport, [2] and can explain the band-like transport of localized charges. [3,4] However, in Marcus theory, the interaction of charge carriers with phonons is only partially considered by λ, and the nuclear tunneling is neglected completely in the high-temperature limit. Our calculation results show that Marcus theory can underestimate the mobility of all systems, while NTAH and TDWPD methods can achieve good agreements with experimental mobilities. This indicates that the nuclear tunneling effect can facilitate the charge transport and is the major cause of high-mobility in those systems. Moreover, the slightly larger TDWPD mobility than NTAH mobility demonstrates that the electronic delocalization effect existed in TDWPD can also facilitate the charge transport.

References

[1] Ostroverkhova O., Cooke D. G., Shcherbyna S., et al, "Bandlike transport in pentacene and functionalized pentacene thin films revealed by subpicosecond transient photoconductivity measurements", *Physical Review B*, 71, (2005), 035204.
[2] Asadi K., Kronemeijer A. J., Cramer T., et al, "Polaron hopping mediated by nuclear tunnelling in semiconducting polymers at high carrier density", *Nature communications*, 3, (2013),1710.
[3] Geng H., Peng Q., Wang L., et al, "Toward quantitative prediction of charge mobility in organic semiconductors: Tunneling enabled hopping model", *Advanced Materials*, 24, (2012), 3568.
[4] Zhang W., Zhong X., Zhao Y., "Electron mobilities of n-type organic semiconductors from time-dependent wavepacket diffusion method: Pentacenequinone derivatives", *The Journal of Physical Chemistry A*, 116, 2012, 11075.

[Poster#35]

Current-voltage Characteristics of Organic Heterostructure Devices with Insulating Spacer Layers

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Main text The dark current density in donor/acceptor organic planar heterostructure devices at a given forward voltage bias can either increase or decrease when an insulating spacer layer is added between the donor and acceptor layers. The dominant current flow process in these systems often involves the formation and subsequent recombination of interfacial exciplex states. If the exciplex recombination rate limits current flow, an insulating interface layer decreases the dark current. However, if the exciplex formation rate limits the current, an insulating interface layer may increase the dark current. We present a device model to describe this behavior, and we discuss relevant experimental data.

[Poster#36]

Broadband Light Absorption Enhancement in Moth's Eye Nanostructured Organic Solar Cells

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A comprehensive study on inverted organic solar cells (OSCs) with a moth's eye nanostructured (MEN) active layer was carried out. Performance of the MEN-based OSCs and corresponding planar control cells, fabricated with blend of poly[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-bA] dithiophene-2, 6-diyl][3-fluoro-2-[(2- ethylhexyl) carbonyl]thieno[3,4-b]-thiophenediyl] (PTB7):[6,6]-phenyl-C70- butyric-acid-methyl-ester ($PC_{70}BM$) was analyzed. Performance of the MEN-based OSCs was optimized by adjusting the height of MEN pattern in the active layer. Our experimental and theoretical results both reveal that the MEN pattern enhances light absorption in the PTB7:$PC_{70}BM$ active layer, especially over the long wavelength region. This leads to a 7.53% increase in short circuit current density and a 6.15% increase in power conversion efficiency over those of the planar control cell.

[Poster#37]

Efficient Organic-inorganic Hybrid Perovskite Solar Cells Fabricated under High Humidity Condition

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A recent rapid emergence of a newcomer in the PV field is the hybrid organic-inorganic halide perovskite solar cell, the conversion efficiency of which have advanced from 3.8% reported in 2009 to a confirmed extremely high efficiency of 20.1% in the late 2014.[1,2] Critical to the solution process is the morphology of the perovskite active layer, since the perovskite crystal formation largely depends on the interfacial energy, solution concentration, precursor composition, solvent choice, and deposition temperature [3-5]. When the fabrication is processed in the ambient condition with high humidity, controlling the film morphology becomes dominant because the water in the air will dissolve or attack the resulting perovskite film during the processing, resulting in a more porous and rough surface film, which will largely degrade the device performance, as shown in Figure 1. In the paper, we provide a variety of controllable perovskite morphologies by employing different fabrication approaches conducted in the ambient atmosphere. We correlate the morphology to the solar cell performance. A bilayer structure, which has a combination of the strengths of the mesoscopic and planar structures, is identified to be essential for realizing high-performance perovskite solar cells with high reproducibility.

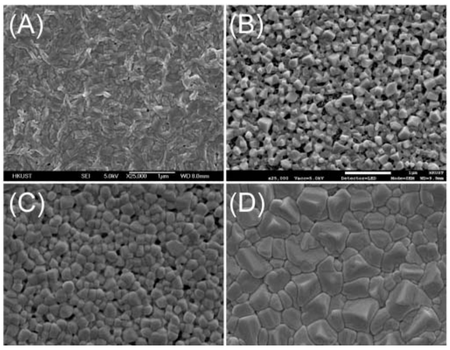

Figure 1. The top-view SEM images of a) PbI2; b) CH3NH3PbI3 film fabricated from the immersion (c) CH3NH3PbI3 film fabricated from the spin coating (d) CH3NH3PbI3 film fabricated from the immersion in the solution, followed by the spin coating.

The the Jsc, Voc, FF, and power-conversion efficiency (PCE) of morphology Figure 1(b) are determined to be 15.9 mA cm-2, 940 mV, 66%, and 9.9%, respectively. A typical device based on Figure 1c is shown with PCE =6.2%, Jsc=11 mA cm-2, Voc=1040 mV and FF=54%. Significant improvement of the Voc is observed, but the rising series resistance calculated from the J-V curve slope at the open-circuit condition gives rise to the lower FF, probably arising from the unreacted PbI2. Meanwhile, the Jsc is also found decreased, suggesting insufficient light absorption and inefficient carrier collection. As expected, the solar cell based on Figure 1d shows a Jsc of 18.5 mA cm-2, Voc of 1058mV and FF of 73.7%, the conversion efficiency is successfully increased up to 14.4%. The highest-performing device based on the bilayer structure achieves a conversion efficiency of 15.2%, with Jsc, Voc and FF of 19.2 mA cm-2, 1060 mV and 74.5% respectively.

References

[1] A. Kojima, K. Teshima, Y. Shirai, T. Miyasaka, *J. Am. Chem. Soc.* **2009**, *131*, 6050.
[2] http://www.nrel.gov/ncpv/
[3] P. Docampo, J. M. Ball, M. Darwich, G. E. Eperon, H. J. Snaith, *Nat. Commun.* **2013**, *4*, DOI 10.1038/ncomms3761.
[4] B. Conings, L. Baeten, C. De Dobbelaere, J. D'Haen, J. Manca, H.-G. Boyen, *Adv. Mater*. **2014**, *26*, 2041.
[5] A. Dualeh, N. Tétreault, T. Moehl, P. Gao, M. K. Nazeeruddin, M. Grätzel, *Adv. Funct. Mater.* **2014**, *24*, 3250.

[Poster#38]

An Insight on Oxide Interlayer in Organic Solar Cells: From Light Absorption and Charge Collection Perspectives

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A comprehensive study of the effect of zinc oxide (ZnO) interlayer on the performance of bulk-heterojunction organic solar cells (OSCs), based on poly[[4,8-bis[(2-ethylhexyl)oxy] benzo [1,2-b:4,5-b'] dithiophene-2,6- diyl] [3-fluoro-2-[(2-ethylhexyl)carbonyl] thieno [3,4-b] thiophenediyl]] (PTB7):3'H-Cyclopropa[8,25] [5,6]fullerene-C70-D5h(6)-3'- butanoicacid, 3'-phenyl-, methyl ester (PC70BM) blend system, is carried out by theoretical simulation and experimental optimization. It is found that a PTB7:PC70BM blend layer thickness optimized for maximum light absorption in OSCs does not generally give rise to the highest power conversion efficiency (PCE). The presence of a ~15 nm thick ZnO interlayer layer between a thinner photoactive layer and the cathode is favorable for efficient OSCs. The ZnO interlayer serves a dual purpose to overcome the Optical-Electrical Mismatch Effect as well as to reduce bimolecular charge recombination. The following three techniques were applied to study the physical mechanisms behind the optical and electrical effects of ZnO spacer: optical admittance analysis, measurement of light intensity dependent current-voltage (I-V) characteristics and transient photocurrent measurements.

[Poster#39]

Theoretical Examination of the Variable Stripe Length Method for Gain Extraction in Polymer Thin Films

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Amplified spontaneous emission (ASE) is widely used to study stimulated emission in an optical gain media. More specifically, variable stripe length (VSL) is the most common method to extract gain coefficients for both inorganic and organic materials [1,2]. Its advantages include simple measurement setup and straightforward data analysis. When used beyond the validity range, however, the result can be misleading, especially for polymer thin films where gain values are relatively low [3].

In this work we theoretically exam the VSL method and the applicability of its assumptions. The VSL method is based on a uniform spatial distribution of state densities inside the excitation stripe where photons follow single pass propagation before collected at the film edge. We use a validated 2-level model to calculate excited state density and photon density on 2-dimensional temporal and spatial scale with variable pump energy [4]. We plot the steady-state distribution in three forms of photon propagation – single pass, double pass (in +/- directions) and double pass with interface reflections which should be the closet scenario to experiments [5]. The result shows that the VSL assumptions can be reached only when excited state density has not been depopulated by activated stimulated emission. The energy dependent saturation is well understood and clearly confirmed by reported measurements [6,7]. For spatial saturation which does not appear in the VSL and is difficult to measure explicitly, however, the photon density at the stripe exit in case of double pass can be an order less than that of single pass. The difference cannot be fully compensated by the modified single pass with a saturation term [3]. The extracted gain may be underestimated by using the VSL method regardless of conditions. This indicates careful validity assessment is important for the VSL method and partly explains why the reported gain values are much less than theoretical expectations of conjugated polymers.

References

[1] R. Dingle, K.L. Shaklee, R.F. Leheny and R.B. Zetterstrom, “Stimulated emission and laser action in gallium nitride”, *Appl. Phys. Lett.*, Vol. 19, Iss. 1, (1971), pp 5-7.

[2] M.D. McGehee, R. Gupta, S. Veenstra, E.K. Miller, M.A. Diaz-Garcia and A.J. Heeger, “Amplified spontaneous emission from photopumped films of a conjugated polymer”, *Phys. Rev. B*, Vol. 58, No. 11, (1998), pp 7035-7039

[3] L.D. Nergo, P. Bettotti, M. Cazzanelli, D. Pacifici and L. Pavesi, “Applicability conditions and experimental analysis of the variable stripe length method for gain measurements”, *Opt. Commun.*, Vol. 229, (2004), pp 337-348.

[4] Y. Xia, “MRes thesis - Quantitatively describing stimulated emission in polymer thin films”, *Imperial College London PE-DTC MRes Archive*, (2014)

[5] U. Ganiel, A. Hardy, G. Neumann and D. Treves, “Amplified spontaneous emission and signal amplification in dye-laser systems”, *IEEE J. Quantum Electron.*, Vol. QE-11, No. 11, (1975), pp 881-892

[6] R. Xia, G. Heliotis, Y. Hou and D.D.C. Bradley, “Fluorene-based conjugated polymer optical gain media”, *Org. Electron.*, Vol. 4, (2003), pp 165-177

[7] R. Xia, P.N. Stavrinou, D.D.C. Bradley and Y. Kim, “Efficient optical gain media comprising binary blends of poly(3-hexylthiophene) and poly(9,9-dioctylfluorene-co-benzothiadiazole)”, *J. Appl. Phys.*, Vol. 111, Iss. 12, 123107, (2012)

Social Activity

Boat Ride to Geopark (High Island, Sharp Island and Yim Tin Tsai Island)

Hong Kong often gives an impression as a metropolitan to its visitors associating with images of tall skyscrapers and busy street scenery. Actually, 40% of the total areas in Hong Kong are designated as country parks. On Day 3 of the Conference, we will show you the other side of Hong Kong in a relaxing boat tour in which we will sail on the sea near Sai Kung. You may enjoy viewing the beautiful waters near HKUST campus and lovely small islands which are also part of Sai Kung Country and Geological Park.

Date: Wednesday, 17 June 2015

Time: 2:30 pm – 6:30 pm

Cost/ Priority: Free but on first-come-first-served basis/ Priority will be given to non-Hong-Kong-based participants.

Enrollment:

[From 14 to 16 June 2015] Sign up at the Registration Desk of the Conference on or before **5 pm of Tuesday, 16 June 2015**

Depart: 2:30 pm from HKUST Pier
Return: 6:30 pm at HKUST Pier

Recommended clothing/stuff to bring:

- Sun protection products (sunglasses, sunscreen, hat, umbrella …etc.).
- Extra water bottle if necessary as some hiking might be required (drinks and light snacks are also available on board).
- Short sleeves and cotton or linen clothes are recommended.

Tour Details:

- The ferry will sail around the Geopark for a close viewing of the volcanic landscape including Po Pin Chau.
- You will disembark on the Sharp Island. You will be able to see interesting rock formation that evident past volcanic activities on the Island.
- You will visit the Yim Tin Tsai Island and experience the ancient Hakka lifestyle. You will also visit a rural catholic church on the Island if time allows.
- The tour is conducted in English. Drinks and light snacks will be available on board.

Attractions:

High Island – Internationally rare acidic polygonal volcanic rock columns

The volcanic rock columns found on High Island region stand as high as 30 meters. They first appeared some 140 million years ago when subterranean magma and volcanoes were active. Whenever there was an eruption, great lava flows gushed out along with scorching volcanic ash. They spread across the ground surface and formed lava layers. During the cooling period, the rock contracted very uniformly and gave rise to the marvelous hexagonal columnar joints seen today.

Judging by its distribution characteristics, these hexagonal rock columns were formed inside a huge caldera. When the lava flow ran rapidly into this recess, just like porridge being poured into a bowl, it created a semi-enclosed environment which was beneficial to slow cooling making it possible for developing these gigantic Rock Columns. This boat trip will enable you to watch this world class Global Geopark and appreciate the grandeur landscape from a close distance.

Sharp Island – an ideal spot to watch samples of igneous rocks and depositional landscape

The island has been always a popular recreation spot for many people during weekends. It has beautiful beach with lucid water. People can enjoy swimming and other light water sports. Many are playing with their dogs.

There is a typical Tombolo existing, which is a natural embankment formed by the wave depositing sandy and stony particles between the beach and an island 200 meters outside the middle of the water. When low tide, the tombolo will appear above water that people can walk across from the beach to the island. But the embankment will be drowned during high tide.

Interesting igneous rocks such as Quartz Monsonite which looks very much like the special bread we called “Pineapple Bun”. Various pyroclastic rocks also gave good evidence of Sharp Island is located at the edge of the caldera.

Yim Tin Tsai Island – a touch of the old Hakka culture

St. Joseph's Chapel

Yim Tin was once the home of these Hakka Indigenous families who came here some 200 years ago. Besides producing sea-salt from the sea water, they also engaged heavily on farming for survival. However, life was tough. When the Italian Catholic Fathers came and help much in improving their life on the little island, people gradually gave up their traditional religion and switch to believe in Christianity.

The current St. Joseph's Chapel was built in Italian Romanesque style, it was completed in 1890, with a school adjacent to it. The chapel is a Grade III historic building. It has been renovated three times, the last being in 2004. The rehabilitation of the abandoned St. Joseph's Chapel received an Award of Merit as part of the 2005 UNESCO Asia-Pacific Heritage Awards. Cardinal Zen held a special mass in the chapel on 7 May 2006. Now there will be special mass being once every year on the first Sunday in the month of May.

Photo Credit: www.walkhongkong.com; http://trailsofacloud.wordpress.com; http://travelinsaikung.org.hk;

General Information and Maps

Wireless Internet Access

1. Wi-fi in Lo Ka Chung Building: "IASGUEST" (Password = ** Removed **)
2. Wi-fi in HKUST campus: "sMobileNet" (Login = iasguest Password = ** Removed **)
3. Wi-fi at public premises and designated tourist spots in town: "GovWiFi"

(For more details, please see http://www.gov.hk/en/theme/wifi/location)

Useful Phone Numbers

Conference Secretary	Telephone Number	Location	Office Hours
Prudence Wong	2358 5061 (On-campus ext. 5061)	IAS2032, 2/F, Lo Ka Chung Building, Lee Shau Kee Campus, HKUST	08:45 - 17:33 (Mon - Fri) (Lunch break: 13:00 - 14:00)

Service or Shops	Telephone Number	Location	Opening Hours
Bank of China	2358 2345	G/F, near the Entrance Piazza and next to Lift 1	09:00 - 17:00 (Mon - Fri) 09:00 - 13:00 (Sat)
Bank of East Asia	3609 2425	G/F, near the Entrance Piazza and next to Lift 4	09:00 - 17:00 (Mon - Fri)
Hang Seng Bank	2998 6262	G/F, near the Entrance Piazza and next to Bank of China	
Bookstore	2358 6400	G/F Entrance Piazza	09:00 - 18:00 (Mon - Sat)
Medical Clinic	2358 6670	LG1010 - LG1028A (via lift 4)	09:00 - 12:30 & 13:30 - 16:45 (Mon - Fri) 09:00 - 11:45 (Sat)
Souvenir Center	2358 6699	G/F Room G027 (across the Piazza)	09:00 - 17:15 (Mon - Fri)
Mailing Services	2358 6333	Room 2615, 2/F (via Lifts 31-32)	09:00 - 12:45 & 14:00 - 17:15 (Mon - Fri) (Closed on Sat, Sun & PH)
Supermarket	2719 1463	LG7 (via Lifts 10-12 / 13-15)	08:30 - 24:00 (Sun - Fri) 08:30 - 21:00 (Sat & PH)

For more information, please visit IAS Information for Visitors website on http://ias.ust.hk/web/ias/eng/visit.php or Campus Services Office website on https://www.ab.ust.hk/cso/.

Local Emergency Telephone Number

Emergency / Ambulance	**999 (outside campus) / 2358 8999 (within campus)**

Choices of meals in the Main Campus

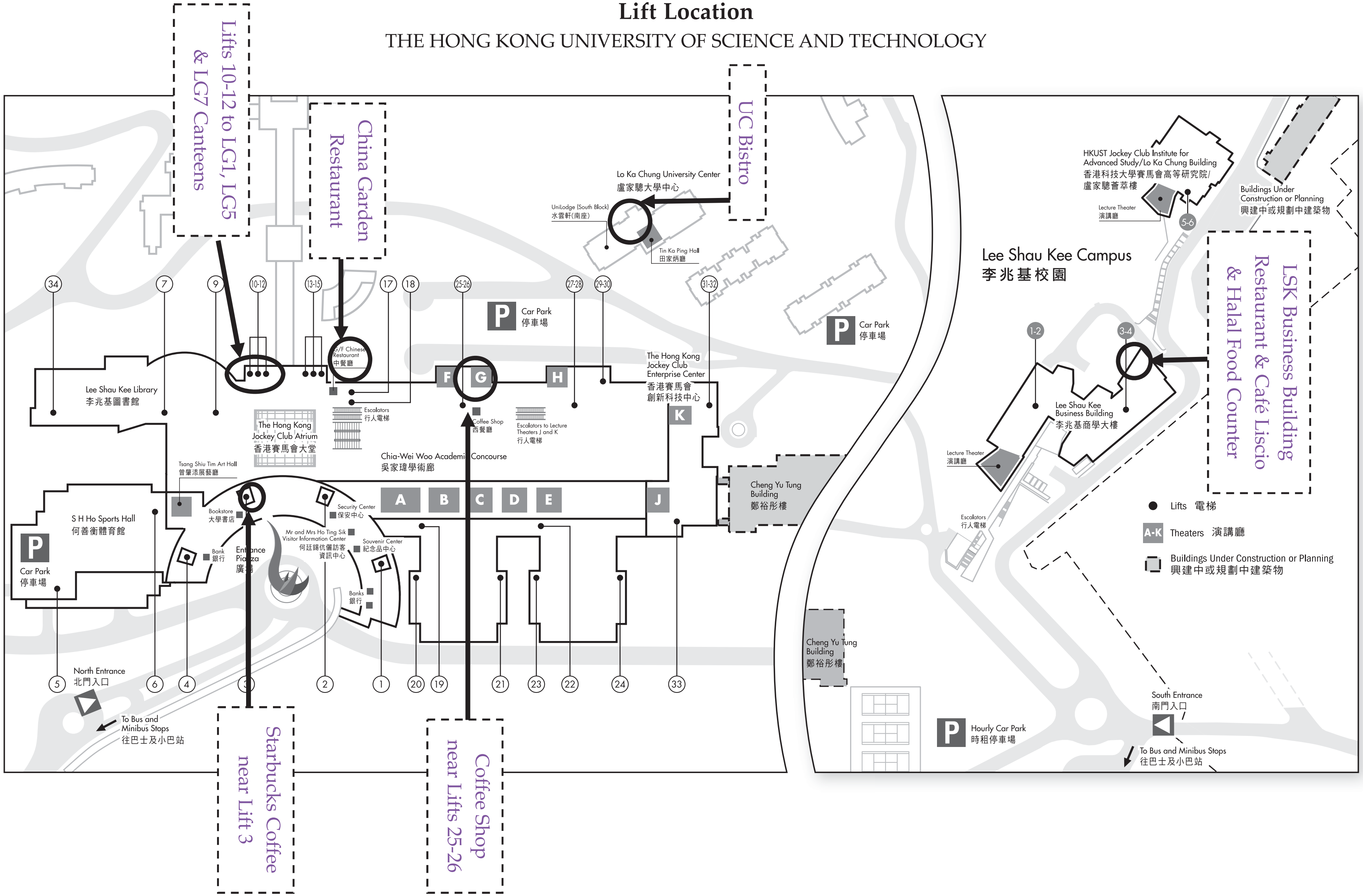
There are a variety of food choices available for breakfast and dinner in the University. Here is the list for your reference.

Remarks: Registered participants will be provided with lunches from 15 to 19 June (both inclusive) at China Garden Restaurant and the dinner banquet on 16 June 2015. Other meals are self-arranged.

Location	Restaurants	Types of Food	Opening Hours
LSK Business Building G/F	**LSK Business Building Restaurant**	Soups, pasta and rice dishes, hot entrees and Chinese barbecue, vegetarian food, snacks, coffee, tea, and soda	07:30 - 21:00 (Mon - Sat) 07:30 - 19:00 (Sat)
	LSK Business Building Café Liscio	Pastry and muffins, Panini, salad, gourmet coffee and smoothies	07:30 - 19:00 (Mon - Sat) 08:00 - 19:00 (Sun & PH)
	Halal Food Counter	Kebabs, Indian curries, biryanis and pizzas	10:00 - 20:00 (Daily) Closed on PH
1/F (near Lifts 25-26)	**Coffee Shop and Coffee Kiosk**	Hot meals, sandwiches, baked potatoes, snacks, pastries, fruits, desserts and drinks	07:30 - 22:30 (Mon - Sat) 10:00 - 18:00 (Sun & PH)
Lo Ka Chung University Center	**UC Bistro & Uni-Bar (For reservations: 2335 1875)**	Western menu, lunch, dinner and snacks	11:00 - 21:30 (UC Bistro) 12:00 - 23:00 (Uni-Bar)
G/F (near Lifts 13-15)	**[Lunch Venue] China Garden Restaurant (For reservations: 2358 1133)**	Chinese dim sum, and Peking & Cantonese dishes	11:00 - 22:00 (Mon - Sat) 10:00 - 22:00 (Sun & PH)
LG1 (via Lifts 10-12 / 13-15)	**LG1 Canteens**	Fast food, sandwiches, snacks and desserts	07:30 - 21:00
LG5 (via Lifts 10-12)	**McDonald's**	Burgers, fast food	07:00 - 24:00 (Daily)
LG7 (via Lifts 10-12)	**Asia Pacific Catering**	Hong Kong and Asian style fast food	07:30 - 21:00 (Mon - Sat) 09:00 - 21:00 (Sun & PH)
LG7 (via Lifts 10-12)	**Gold Rice Bowl Delicious Food**	Japanese and South East Asian style food	11:00 - 21:00
LG7 (via Lifts 10-12)	**Milano Fresh**	Western style fast food and Italian gourmets	11:00 - 21:00
Atrium	**Starbucks Coffee**	Pastry, muffins and gourmet coffee	08:00 - 21:00 (Mon - Fri) 08:30 - 20:00 (Sat & Sun)

Lift Location

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY



Bad Weather Arrangements for On-campus Administrative Offices and Programs

- "Bad weather" here refers to the adverse weather condition that leads to the issue of Rainstorm and/or Tropical Cyclone Warning Signals by the Hong Kong Observatory (HKO).
- In general, **Signal No.8** of Tropical Cyclone Warning System and/or **Black Signal** of Rainstorm Warning System will lead to closure of most administrative offices, and suspension or cancellation of Programs.
- For details of both Warning Signals, please refer to HKO website:-

Hong Kong's Tropical Cyclone Warning Signals:
http://www.hko.gov.hk/publica/gen_pub/tcws.pdf
Rainstorm Warning System: http://www.weather.gov.hk/wservice/warning/rainstor.htm#

Please see below for the possible situations and arrangements:-

Situations	**Arrangements***
When HKO announces one or more of the following: ● Signal No. 1 or No. 3 in Tropical Cyclone Warning System, and/or ● Amber or Red Signal in Rainstorm Warning System	All offices will operate and scheduled programs will be held **as usual**.
When HKO announces ● the No. 8 signal in Tropical Cyclone Warning System will be hoisted within 2 hours (pre-No.8), and/or ● the Black Rainstorm Warning is issued.	● Most offices will be closed and programs will be cancelled. ● All should stay indoors wherever they are and do not leave until the warning is cancelled and the conditions are safe.
If HKO announces that the No. 8 signal or the Black Rainstorm Warning is cancelled:- (a) At or before 06:30	(a) Offices will operate as usual while programs starting **at or after 08:30** will be held as scheduled.
(b) At or before 14:00	(b) Offices and Programs will **resume** their operation/running **in two hours** after the cancellation of the signal/warning.
(c) At or after 14:00	(c) Offices will be closed until end of the day. **All** programs of the day will be **cancelled**.

** All arrangements are indicative and subject to changes with the consideration of actual situations.*

Walking Routes from Bus Stations
to HKUST Jockey Club Institute for Advanced Study
(Lo Ka Chung Building)

Bus:
91M→Po Lam 寶林
91→Clear Water Bay
清水灣
792M→Tseung Kwan O / Sai Kung
將軍澳/ 西貢
Minibus:
11M→Hang Hau 坑口
12→Po Lam / Sai Kung
寶林/ 西貢

Bus:
91/91M→Diamond Hill
鑽石山
91P→Choi Hung 彩虹
Minibus:
11→Choi Hung 彩虹
104→Ngau Tau Kok
牛頭角

Legend

🚕	Taxi Station 的士站
$	Bank & ATM 銀行及提款機
ATM	ATM 提款機
🚌	Bus /Minibus Station 巴士及小巴站
● ●	Lift Number 升降機號碼
■	Lecture Theater 演講廳

LOCATION MAP

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY

MTR Stations with bus or green minibus service to HKUST 提供往科大巴士或綠色專線小巴服務的港鐵車站		
Diamond Hill 鑽石山：	🚌 91, 91M	
Choi Hung 彩虹：	🚌 91, 91M	🚐 11, 11S
Ngau Tau Kok 牛頭角：		🚐 104
Tiu Keng Leng 調景嶺：	🚌 792M	
Hang Hau 坑口：		🚐 11, 11M, 11S
Po Lam 寶琳：	🚌 91M	🚐 11S, 12

Transportation from airport to HKUST:

For passengers with bulky luggage, taking a taxi to HKUST direct is recommended.
Those with simple luggage may take Airport Bus A22 to Lam Tin, and change for taxi to HKUST.

🚌 **Bus Routes 巴士路線**

🚐 **Green Minibus Routes 綠色專線小巴路線**

11th International Conference on Optical Probes of Conjugated Polymers and Organic Nanostructures (OP 2015)

One-page Conference Schedule

	Monday	Tuesday	Wednesday	Thursday	Friday
	15-Jun	16-Jun	17-Jun	18-Jun	19-Jun
08:50 - 09:00	Conference Opening				
	Session M1 (KS Wong)	Session Tu1 (Akshay Rao)	Session W1 (Valy Vardeny)	Session Th1 (Zhigang Shuai)	Session F1 (Charles Surya)
9:00	Plenary #01: Donal Bradley	Plenary#16: Lewis Rothberg	Plenary#33: Guglielmo Lanzani	Plenary#41: Yuguang Ma	Invited#59: He Yan
9:15					
9:30					Invited#60: Lingyi Meng
9:45	Invited #02: Davide Comoretta	Invited#17: Kirk Schanze	Invited#34: Ji-seon Kim	#42: Fernando B Dias	
10:00				Invited#43: Feng Li	#61: Alex J Barker
10:15	Invited #03: Ruidong Xia	Invited#18: Martin Vacha	#35: Artem A Bakulin		#62: Johannes M Richter
10:30			#36: Florian Steiner	#44: Przemyslaw Data	**Coffee Break**
10:45	**Coffee Break**	**Coffee Break**	**Coffee Break**	**Coffee Break**	
11:00					Session F2 (KS Wong)
	Session M2 (Howe-siang Tan)	Session Tu2 (Lewis Rothberg)	Session W2 (Annamaria Petrozza)	Session Th2 (Patrick Parkinson)	Invited#63: Charles Surya
11:15	Invited#04: Chihaya Adachi	Invited#19: Vivian Yam	Invited#37: Changqin Wu	Invited#45: Zhigang Shuai	
11:30					#64: Milan Vrućinić
11:45	Invited#05: Andy Monkman	Invited#20: Bin Liu	#38: Justin Hodgkiss	#46: Linda Peteanu	#65: Zengqi Xie
12:00			#39: Yin Song	Invited#47: Wenjing Tian	#66: Jasmine Rivett
12:15	#06: David Graves	#21: Marc Etherington	Invited#40: Yi Zhao		Conference Closing
12:30	**Lunch**	#22: Hameed A Al Attar		**Lunch**	**Lunch**
12:45		**Lunch**	**Lunch**		
13:00					
	Session M3 (Andy Monkman)			Session Th3 (Kok Wai Cheah)	
14:00	Invited#07: Howe-siang Tan	Session Tu3 (Jiannong Wang)	Boat Trip	Invited#48: Shihe Yang	
14:15		Invited #23: Annamaria Petrozza			
14:30	Invited#08: Margherita Maiuri			#49: Ajay Ram Srimath Kandada	
14:45		Invited#24: Furong Zhu		Invited#50: Wallace C H Choy	
15:00	Invited#09: Carlo Silva				
15:15		#25: Xuhui Zhu		#51: Shu Kong So	
15:30	Invited#10: Franky So	#26: Andreas C Jakowetz		Invited #52: Yuanping Yi	
15:45		Invited#27: Sergei Tretiak			
16:00	**Coffee Break**			**Coffee Break**	
16:15		**Coffee Break**			
	Session M4 (Carlo Silva)			Session Th4 (Shihe Yang)	
16:30	Invited#11: Valy Vardeny	Session Tu4 (Martin Vacha)		Invited#53: Patrick Parkinson	
16:45		Invited#28: Jiannong Wang			
17:00	#12: Frédéric Laquai			#54: Kai Chen	
17:15	Invited#13: Akshay Rao	#29: Eitan Ehrenfreund		#55: Juliane Gong	
17:30		Invited#30: Shijie Xie		Invited#56: Kok Wai Cheah	
17:45	#14: Panagiotis Keivandis				
18:00	Invited#15: Jang-joo Kim	Invited#31: Chongan Di		#57: Andrew Musser	
18:15				#58: Felix Deschler	
18:30	Conference Reception and Poster Session until 20:00	#32: Jack Wildman			
18:45		Conference Banquet until 21:30			

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