# Fundamental Properties and Industrial Applications of Nanostructured Materials: Wrinkled Graphene and Hydrogen-adsorbing Porous Materials

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We first report the wrinkling behavior of monolayer graphene on soft polydimethylsiloxane (PDMS) substrate under a uniaxial compressive strain. Graphene is grown by thermal chemical vapor deposition, and then transferred on the prestretched PDMS. As the applied strain is varied, the wavelength and the amplitude of the wrinkle are measured with an atomic force microscope. The cross-section of the system is probed using a transmission electron microscope. We observe the evolution of the wrinkle pattern and the transition from a simple sinusoidal to a complex folding configuration as increasing the compressive strain. Bifurcation (period doubling) of the wrinkle pattern is found to occur repeatedly. We propose a theoretical model to describe and understand the evolution of the wrinkle configuration of the system.

We then present our work to achieve molecular hydrogen storage in nanomaterials that can function under practical vehicle-operation conditions. On the theoretical side, we carry out first-principles electronic and atomic structure calculations to search for porous materials decorated with extra metal atoms to bind hydrogen molecules. Contributions of so-called “Kubas” interactions as well as dipole interactions to the molecular hydrogen binding are investigated and the influences of spin states on the stability of the adsorption are examined. On the experimental side, introducing organo-metallic precursors (OMPs) is found to be an important step in the synthesis process. Metal organic frameworks and silica are studied as scaffold materials on which transition metal atoms are doped. When methyl aluminoxane reacts with silica, OMPs are easily attached to the system and the hydrogenation gives rise to the replacement of organic ligands with hydrogen. Molecular hydrogen storage through Kubas interactions has been confirmed using the Temperature Programmed Desorption experiment. Other possible materials such as carbide-derived carbon, porous metal hydrides, and graphene-based composite materials are proposed as well.