Doping Effect and Electron-Hole Asymmetry in Cuprates

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Motivated by recent STM observation, we investigate the microscopic effects of doping in charge-transfer insulators. We demonstrate that introducing holes into the system gives rise to in-gap bound states, which originate from localized Zhang–Rice singlets. This observation further inspires us investing the Antiferromagnetic (AFM) order in the cuprates. We revisit this regime within the three-band Emery model using a coordinated set of many-body calculations—variational Monte Carlo (VMC), determinant and auxiliary-field QMC (DQMC/AFQMC), density-matrix embedding theory (DMET), and Gutzwiller-type approaches (GA). With parameters constrained to reproduce the experimentally observed parent-compound superexchange J and related benchmarks, we map the AFM phase boundary as a function of doping. We further examine parameter dependencies—e.g., the charge-transfer energy Δ, t_{pd}, and t_{pp}—and assess the sensitivity of AFM order to experimentally relevant conditions. Our results offer fresh insights into the interplay between dopants and localized holes, shedding light on the fundamental physics of lightly hole-doped cuprates and their evolution toward metallic or superconducting states.