Nagoya University

Plaform: Nano/Energy

RCMS Research Center for Materials Science, Nagoya University

Theoretical Chemistry Colloquium

June 6, 2013 (Thu), 16:00-17:00

RCMS, 2nd floor, Chemistry Gallery

Disorder and excitonic structure in organic semiconductors

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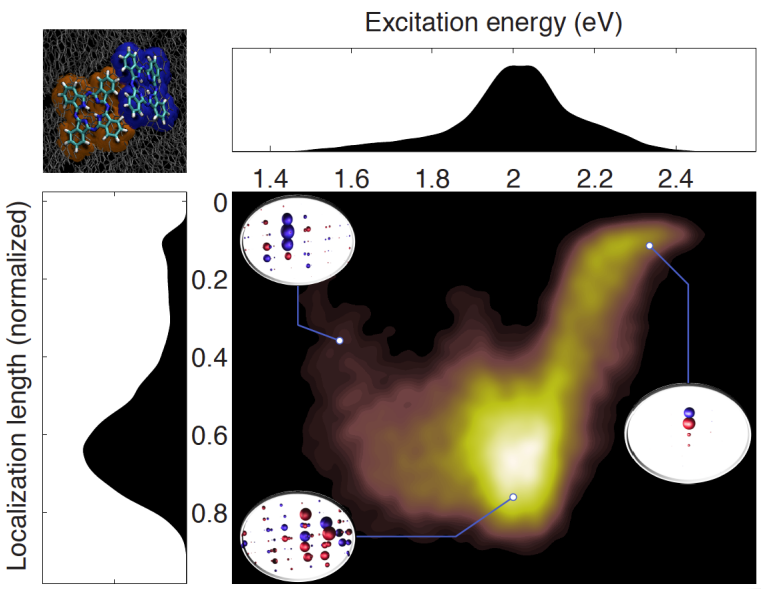
Abstract: *A two-pronged computational study using both atomistic calculations and analytic models has revealed insights into how disorder affects the electrical and optical properties of organic semiconductors. First, the effects of thermal fluctuations and impurity doping in the exciton band structure of room temperature metal-free phthalocyanine (H2Pc) crystals was studied. Thermodynamically accessible microstates were sampled explicitly from all-atom molecular dynamics simulations, and the structure of excitonic states were determined using a hybrid quantum mechanical/molecular mechanical (QM/MM) calculations using time-dependent density functional theory (TDDFT). The density of states shows evidence of thermally-induced dynamical localization due to collective interactions beyond the nearest neighbor level. Second, disorder-induced localization transitions in tight binding Anderson models were revisited. Using newly developed notions of partial freeness in random matrices, the density of states can be approximated accurately with known error bounds and without requiring explicit calculation of eigenvectors. An accurate approximation was found that reproduces the first seven moments of the density of states accurately, with an error that grows only linearly with the number of neighbors on a lattice.*



[1] JC and Alan Edelman, Partial freeness of random matrices. arXiv:1204.2257
[2] JC, Eric Hontz, Jeremy Moix, Matthew Welborn, Troy Van Voorhis, Alberto Suárez, Ramis Movassagh, and Alan Edelman. Error analysis of free probability approximations to the density of states of disordered systems. Phys. Rev. Lett. 109 (2012), 036403. arXiv: 1202.5839

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