Mesoscale Priority Research Direction: **Modeling of electronic dynamics and transport at multiple time- and length-scales**

Opportunity

Research and discovery utilizing the approaches of theory, modeling, and simulation from nano-building blocks (e.g., nanotubes, quantum dots, clusters, and nanoparticles), to complex nanostructures and nano-interfaces, and to their assembly/growth into complex electronic device architectures (i.e., the bottom up approach, from nano- to mesoscale). Current absence of quantitative theoretical methods that describe newly observed phenomena increasingly limits our progress to assemble nano-sized blocks promising new physics into functional meso-scale devices, sensors, etc.

Meso Challenge

Need of quantitative theoretical tools for

- Discovery of novel functionalities and emerging phenomena resulting from competing interactions;
- Simulation of long-range transport of charges and energy;
- Modeling and characterization of collective behavior of components and defects;
- Impact of conformational disorder and interfaces on materials functionality and electronic properties;
- Modeling of material's aging at multiple length-scales.

Approach

- Integration of first principle approaches with classical molecular dynamics and coarse-graining models including Monte Carlo-like techniques (interfacing 'quantum' and 'classical' worlds). Example: QM/MM approaches;
- Going beyond Born-Oppenheimer approximation for modeling of electronic and photoinduced dynamics;
- Co-Design strategy for functional meso-materials, and connection to experiments;
- Taking an advantage of the next generation high performance (Exa-Scale) computing;
- Development of materials inverse engineering principles.

Impact

- A quantitative understanding of matter from molecular to nano- to meso- lengthscales, and dynamics from fs to ps to ns to ms;
- Quantitative prediction of novel functionalities emerging from competing interactions;
- Development of 'cheap' computational/ modeling framework vs. common 'expensive' experimental R&D approach.

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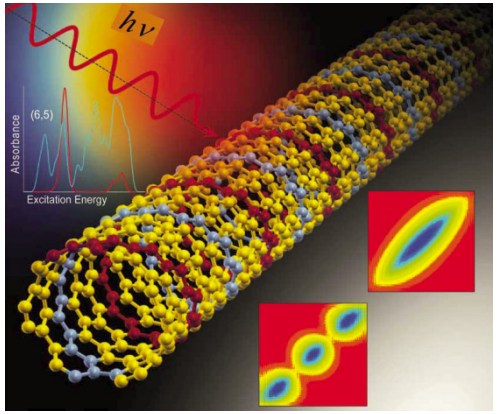
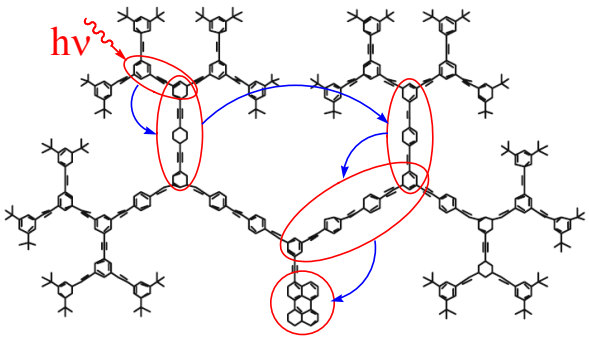
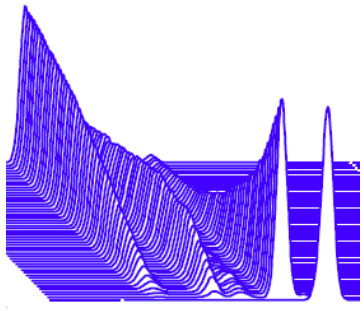
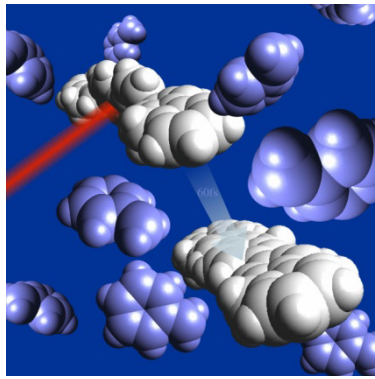


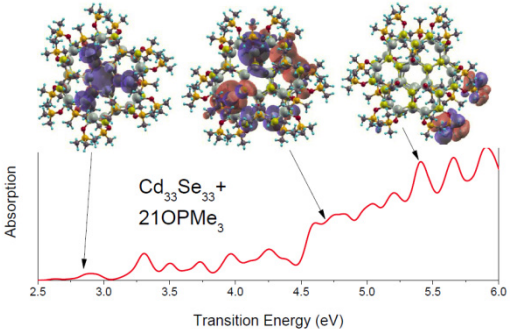






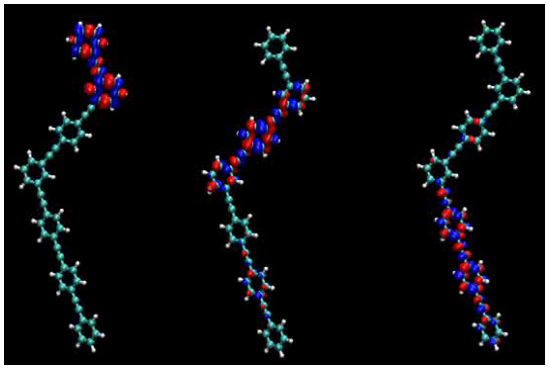
Photoinduced dynamics beyond Born-Oppenheimer approximation

J. Clark, et al, Nature Physics, (2012, ASAP)



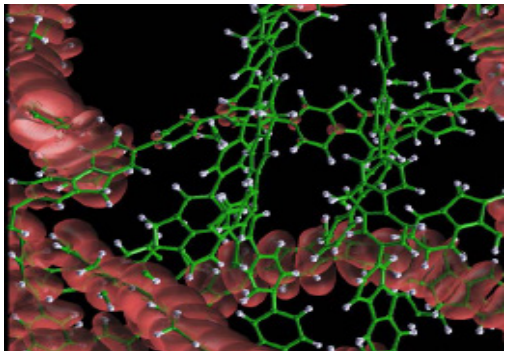
Optical spectra and properties of excited states:

S. Tretiak, Nano Lett., 7, 2201 (2007); S. Kilina, et al, J. Am. Chem. Soc., 131, 7717 (2009)



Charge and energy transfer

S. F. Alberti, et al, J. Phys. Chem. Lett., 1 2699 (2010).



Conformational structure-electronic properties relationships

S. Kilina, et al, ACS Nano 2 1381 (2008).