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Mini lecture series on materials for energy research:

1) Title: "From engineering interfaces in soft electronic materials to efficient perovskite photovoltaics"
   Date: Wednesday, May 13
   Time & Location: 12:00 pm, SSL

   Abstract: 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 organicorganic 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 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.

   Refs: Science, 347, 522 (2015); Advanced Science, 2015, DOI: 10.1002/advs. 201500024

2) Title: "Multiscale DFT-based modeling of functional electronic materials"
   Date: Monday, May 18
   Time & Location: 12:00 pm, SSL

   Abstract: Ever growing complexity of nanomaterials requires robust and predictive multiscale approaches for their theoretical description. Combined with thorough experimental studies such approaches should provide estimates of physical properties of nanostructured materials and enable a rational design of devices. From this perspective I will first briefly discuss merits and drawbacks of time-dependent density functional theory (TDDFT) for calculation electronic excitations in large molecular system, being the only numerically feasible first principle-based approach. I will further

exemplify modeling of several systems: 1). Small-molecule bulk-heterojunction organic solar cells and push-pull chromophores for tunable-color organic light emitters. The emphasis is on electronic processes involving intra- and intermolecular energy or charge transfer driven by strong electron-phonon coupling inherent to pi-conjugated systems. 2). Chemical functionalization of single-walled carbon nanotubes which locally alters the piconjugated network of the nanotube surface and leads to a spatial confinement of the electronically excited wavefunctions. This suggests that enhanced photoluminescent efficiency of semiconducting carbon nanotube materials can be achieved via selective chemical functionalization.
Refs: Chem. Rev. (June 2015 to appear)

3) Title: "Non-adiabatic excited state dynamics simulations of extended molecular systems"
Date: Wednesday, May 27
Time & Location: 12:00 pm, SSL
Abstract: Modelling of non-adiabatic dynamics in extended molecular systems and solids is a next frontier of atomistic electronic structure theory. The underlying numerical algorithms should operate only with a few quantities (that can be efficiently obtained from quantum chemistry), provide a controlled approximation (which can be systematically improved) and capture important phenomena such as branching (multiple products), detailed balance and evolution of electronic coherences. This talk will overview recently developed theoretical methodologies applicable for simulating large molecules underlying an efficient Non-Adiabatic Excited State Molecular Dynamics (NA-ESMD) framework incorporating non-adiabatic quantum transitions. Our calculations of several molecular systems show intricate details of photoinduced vibronic relaxation and identify the conformational degrees of freedom leading to ultrafast dynamics and energy transfer. This theoretical modeling allows us to understand and to potentially manipulate energy transfer pathways in molecular materials suitable for solar energy conversion.
Refs: Acc. Chem. Res., 47 1155 (2014); Nature Comm., 4 2144 (2013)