

# Carnegie Mellon University

## Materials Science & Engineering

presents

### Toward Computational Design of Cluster-Based Functional Nano-Structures

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**Abstract** - Computational materials design offers tremendous potential for discovery and innovation. This powerful concept relies on computational exploration of the vast configuration space of materials structure and composition to identify promising candidates with desired properties for target applications. In fact, many applications do not rely on a single material but on the combination of several materials in a functional nano-structure. Examples for functional nano-structures include the dye-oxide interface, at which charge separation is achieved in dye-sensitized solar cells, and nanocatalysts based on clusters dispersed on a large surface area support. Therefore, we would like to design not just a material, but a functional nano-structure. This requires the combination of accurate electronic structure methods with efficient optimization algorithms. The electronic properties and the resulting functionality of a nano-structure cannot be deduced directly from those of its isolated constituents. Rather, they emerge from a complex interplay of quantum mechanical interactions that depend on the local environment at the nano-scale. Describing these effects requires a fully quantum mechanical first principles approach. In the first part of the talk, many-body perturbation theory within the  $GW$  approximation, where  $G$  is the one-particle Green's function and  $W$  is the screened Coulomb interaction, is used to elucidate the size effects in the energy level alignment at the interface between dye molecules and  $\text{TiO}_2$  clusters of increasing size [1,2]. In the second part of the talk, a new approach is presented for computational design of clusters using property-based genetic algorithms (GAs). These algorithms perform optimization by simulating an evolutionary process, whereby child structures are created by combining fragments ("mating") of the fittest parent structures with respect to the target property. Property-based GAs tailored to search for low energy, high vertical electron affinity (VEA), and low vertical ionization potential (VIP) are applied to  $\text{TiO}_2$  clusters with up to 20 stoichiometric units. Analysis of the resulting structures reveals the structural features associated with a high VEA and a low VIP and explains the absence of the expected size trends [3,4].

**Bio** - Noa Marom received a B.A. in Physics and a B.S. in Materials Engineering, both *Cum Laude*, from the Technion- Israel Institute of Technology in 2003. From 2002 to 2004 she worked as an Application Engineer in the Process Development and Control Division of Applied Materials. In 2010 she received a Ph.D. in Chemistry from the Weizmann Institute of Science. She was awarded the Shimon Reich Memorial Prize of Excellence for her thesis on describing the electronic structure of organic semiconductors from first principles. She then pursued postdoctoral research at the Institute for Computational Engineering and Sciences (ICES) at the University of Texas at Austin. In 2013 she joined the Physics and Engineering Physics (PEP) Department at Tulane University as an Assistant Professor. Her field of research is computational materials science. She is working toward computational design of materials, interfaces, and nanostructures for applications in *e.g.*, photovoltaics and catalysis.

**Doherty Hall 2210, 11:30AM**  
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