

# SEMINAR

Research Talks from the Resnick Fellows



**RESNICKINSTITUTE**  
science + energy + sustainability



**Allegra L.  
Liberman-Martin PhD**

Resnick Postdoctoral Scholar

## Side Chain Design in Brush Block Copolymer Photonic Crystals

Brush block copolymers feature polymeric side chains grafted to a linear backbone, and these materials display interesting properties due to their dense functionality, low entanglement, and ability to rapidly assemble to highly ordered nanostructures. Using ruthenium-catalyzed ring opening metathesis polymerization (ROMP), our group has prepared brush block copolymers that self-assemble to photonic crystal films. Previous work has shown that the frequency of light reflected can be tuned from the visible to the near-infrared regime by varying the backbone length or blending in polymeric additives. However, the impact of side chain properties on self-assembly and photonic behavior remains poorly understood. My talk presents a series brush block copolymers featuring side chains with low glass transition temperatures. The photonic properties, self-assembly, and morphologies of these materials will be discussed.



**Yuanyue  
Liu PhD**

Resnick Postdoctoral Scholar

## Predictive Modeling of Materials for Electronic and Energy Applications

Advances in materials have continuously revolutionized our lives. These advances can be accelerated with the help of theory and simulations. In this presentation, I will discuss some examples, in which we use theory and simulations to understand, predict and design low-dimensional nanomaterials (e.g. nanotube, graphene, and atomically-thin metal dichalcogenides) for electronics and energy applications. These materials have attracted great interest due to their intriguing properties and promising applications, yet they still face many challenges to reach their full potential.

I will present our understanding and predictions of how to synthesize materials with desired properties (including theory-guided synthesis of novel materials), how to tune the defects to optimize material performance, and how to engineer the interface for better transport of charge carriers, all of which are important for electronic/optoelectronic applications. I will also show how the surface electronic structure controls the atom's adsorption, on which we derived a model that has helped explained a number of experiments and guided the discovery of new materials for energy storage.

3:00 to 4:00 pm | Wednesday, 3/8/17  
Guggenheim 101 | Lees-Kubota Lecture Hall  
Caltech Campus | [resnick.caltech.edu](http://resnick.caltech.edu)

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