

Extreme Thin Film Material Simulations

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Seminar host: Adarsh Krishnamurthy**

Abstract

Thin film materials have a wide range of applications in modern technologies, ranging from surface coatings, electronic/optoelectronic devices, MEMS, to thin film solar cells and batteries/ultracapacitors. These thin film materials are extremely diverse in their physical dimensions, chemical compositions, and fabrication processes, thereby imposing grand challenges in modeling and simulation aiming toward elucidating material properties as well as optimization of fabrication protocols. In this talk, I will present our recent applications of multiscale molecular simulations on thin film materials over several extrema in the spectrum of film dimensions, compositions, processing conditions, and energy scales:

- Film dimension: one-atomic-layer thick graphene vs. hundreds of nanometer thick thin film solar cells.
- Chemical compositions: inorganic vs. organic or organic-inorganic hybrid materials.
- Process conditions: vacuum deposition vs. solution processing.
- Energy scales: 0.02 eV (room temperature) vs. 10 keV in FIB.

By utilizing molecular simulation techniques across both spatial (up to hundreds of nanometers) and temporal scales (up to seconds), the structural details and evolution that are difficult to be characterized from current state-of-the-art experimental techniques can be revealed. Therefore, we demonstrate that multiscale molecular simulations can help fill the gap between fabrication conditions and material performances, and pave the way towards the optimization of material structures as well as fabrication processes of advanced thin film materials.

Bio

Dr. **Chun-Wei Pao** is currently an Associate Research Fellow in Research Center for Applied Sciences (RCAS), Academia Sinica, Taiwan. He received his Bachelor's degree from Department of Power Mechanical Engineering at National Tsing Hua University in Taiwan in 1996, Master's degree from Institute of Applied Mechanics at National Taiwan University in 2001, and Doctor of Philosophy degree at Department of Mechanical and Aerospace Engineering at Princeton University in 2007. After receiving his Ph.D. degree at Princeton, he worked at Theoretical Division in Los Alamos National Laboratory as a post-doctoral research associate from 2007 to 2009. Dr. Pao joined the faculty of RCAS in November, 2009, and was promoted to Associate Research Fellow in May, 2014. Dr. Pao has worked extensively on multiscale simulations of materials ranging from solid to soft matter materials, and has published papers on leading journals such as Nano Letters, Physical Review Letters, and Energy & Environmental Sciences. Dr. Pao has received Academia Sinica Career Development Award in 2016, and the Young Theorist Award from the National Center for Theoretical Science, and the Youth Award in 2014.

This seminar counts towards the ME 600 seminar requirement for Mechanical Engineering graduate students.

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