Materials Science and Technology Division

# "Surface and Interface at Nanoscale: From $C_{60}$ to Transition-Metal Nanoparticles"


## Dr. Lin-Lin Wang
## University of Illinois at Urbana-Champaign


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**Abstract:**

Materials of nanometer size have brought exciting new functionality. Two such examples are $C_{60}$ on noble metal surfaces that serve as potential molecular electronic devices and transition-metal nanoparticles (NP) that are effective catalysts in hydrogen fuel cells. At the nanoscale, surface and interface dominate the properties of these systems. I will present first-principles calculations that directly explain experimental observations and predict new behavior of supported $C_{60}$ and transition-metal NPs. For the seemingly simple $C_{60}$-metal interface, there are a few surprises regarding the abnormal work function change and surface vacancy induced by the $C_{60}$ self-assembly. For transition-metal NPs, a range of structural properties arising from surface and interfaces will be discussed. In particular, a simple correlation and its electronic origin for core-shell preference in bimetallic NPs are revealed. For NPs acting as catalysts in working condition, effects from support and passivation by small molecules are inevitable. I will discuss such effects on the structure of supported Pt and PtRu NPs in terms of bulk-like metal-metal bond length and inhibition of shear instability by hydrogen passivation.


Host: David Singh (241-1944, singhdj@ornl.gov)