

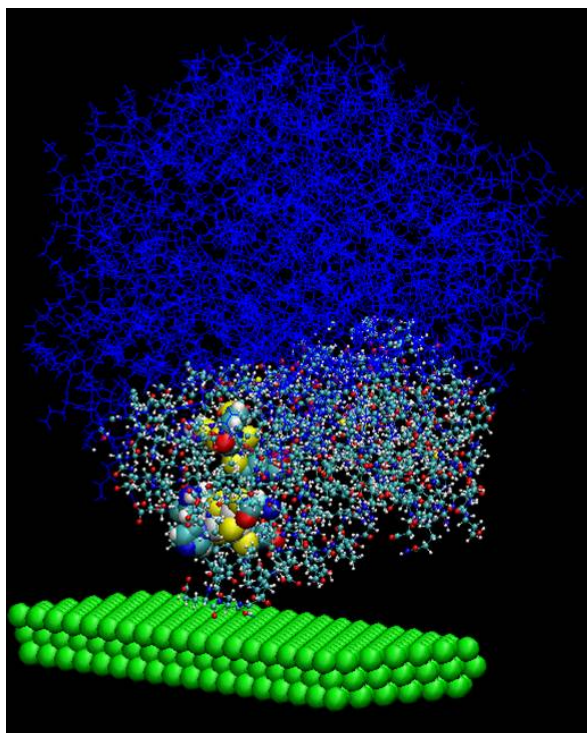
THE GEORGE WASHINGTON UNIVERSITY
Department of Physics
Summer Colloquium

**Molecular Interactions with Energy
Nanostructures - from Fundamental Design
to System Development**

Prof. Z. Xiao Guo

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Mitigating climate change and ensuring energy security demand clean energy solutions, such as the use of hydrogen as an energy carrier, energy harvesting from biological sources, and the removal of CO₂ from fossil fuels. Development of such solutions requires a fundamental understanding of the electronic structure and the nature of bonding, as well as practical control of compound structures. Close integration of fundamental and applied research activities offer a unique capability in the search for effective industrial solutions. First-principles simulations on carbon nanostructures show the importance of defects and doping on extra hydrogen uptake, and a small change of C-C interspacing on the “mode-switching” of hydrogen sorption. Similar studies on the 3d Transition Metal (TM) series (Sc to Fe) doped borazine (B₃N₃H₆) demonstrate that appropriate doping can lead to hydrogen release without the emission of unwanted NH₃. A new desorption path for the (Li NH₂ + Li H) was identified for further design of this promising hydrogen storage reaction couple. Simulations on catalytic enzymes clearly indicate hydrogen diffusion paths and electron transfer mechanisms for the design of effective biological fuel cells. More recently, we have identified an effective system for CO₂ activation and capture, and developed a hydrogen storage system that can release pure hydrogen below 100°C, ideal for fuel-cell powered vehicles and portable devices. Comparison is made with experimental developments where possible.



*Multiscale simulations of enzyme interaction
with an electrode surface.*

TIME: 12:00-1:00 pm, Wednesday, June 17, 2009

PLACE: 104 Corcoran Hall, GWU

725 21st Street, N.W. (Between G and H Streets)

METRO STATION: GWU/FOGGY BOTTOM (BLUE & ORANGE LINES)