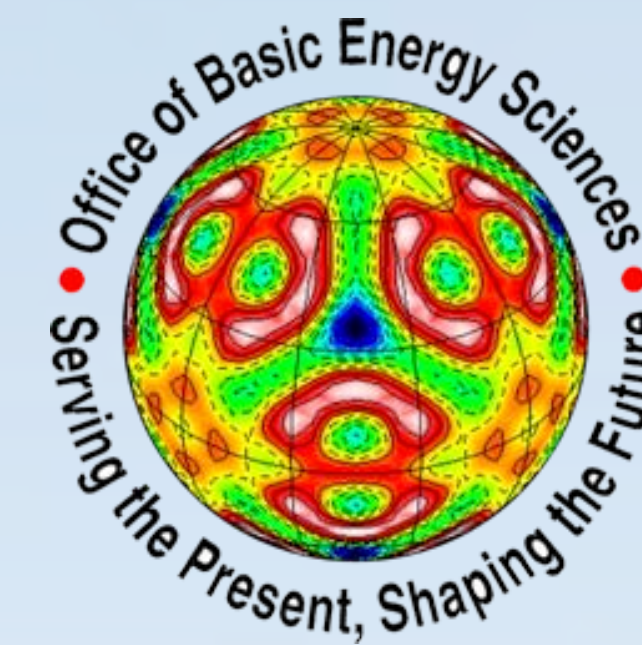




Office of Science  
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U.S. DEPARTMENT OF  
**ENERGY**



**3<sup>rd</sup> ANNUAL COORDINATION MEETING OF THE DOE  
COMPUTATIONAL MATERIALS AND CHEMICAL SCIENCE NETWORK (CMCSN) ON  
“PREDICTIVE MODELING OF THE GROWTH AND PROPERTIES OF ENERGY-RELEVANT THIN FILM AND  
NANOSTRUCTURES”**

**January 20 – 22, 2011**

**Room 3.204, Natural Science and Engineering Research Laboratory (RL), University of Texas at Dallas, TX**

CMCSN Coordinators: Kai-Ming Ho (Iowa State U & Ames Lab) Zhenyu Zhang (U Tennessee)

Scientific Committee: Chair: Yves Chabal (UT Dallas)  
KJ Cho (UT Dallas); Bob Helms (UT Dallas); David Langreth (Rutgers U)  
Kai-Ming Ho (ISU); Cai-Zhuang Wang (Ames Lab); Zhenyu Zhang (U Tennessee)

## Program

### Thursday January 20

**2:00-2:30 pm**      **Opening remarks & welcome**      Yves Chabal and Bob Helms

**Session I**      **Nonequilibrium Growth**      Chair: K.J. Cho (UT Dallas)

2:30-3:00 pm      *Ted Einstein*      - Ordering of giant molecular honeycomb networks: closed-shell quantum dots or metallic surface states?  
(U Maryland)

3:00-3:30 pm      *Jim Evans*      - Far-from-equilibrium growth of epitaxial metal nanostructures in multicomponent systems: Predictive atomistic modeling  
(Ames Lab/ISU)

3:30-4:00 pm      *Feng Liu*      - Non-equilibrium compositions of alloy quantum dots and its correlation with growth mode  
(U Utah)

**4:00-4:20 pm**      **Coffee Break**

**Session II**      **Graphene**      Chair: Michael Tringides (ISU)

4:20-4:50 pm      *Phil First*      - Quantized states of electrons in epitaxial graphene  
(Georgia Tech)

4:50-5:20 pm      *Myron Hupalo*      - Metals on graphene: preparation and growth  
(Ames Lab)

5:20-5:50 pm      *Cai-Zhuang Wang* - Adsorption of metal atoms on graphene by first-principles calculations  
(Ames Lab)

**6:00 pm**      **Reception and pizza** (Remarks by Mark Spong, Dean of the Erik Jonsson School of Engineering)

### Friday January 21

**Session III**      **Water on Surface**      Chair: Yves Chabal (UT Dallas)

8:30-9:00 am      *Adri van Duin*      - Development and application of ReaxFF reactive force fields to model surface chemistry  
(Penn State)

9:00-9:30 am      *Peter Feibelman*      - Structure of water monolayers on close-packed precious metals  
(Sandia)

9:30-10:00 am      *Annabella Selloni*      - Structure, defects and water adsorption on TiO<sub>2</sub> surfaces  
(Princeton U)

**10:00-10:30 am**      **Coffee Break**

- Session IV Metal on Semiconductor** Chair: Zhenyu Zhang (U Tennessee)
- 10:30-11:00 am *Pat Thiel* (Ames Lab/ISU) - Ag on Si(111): An Old System with New Surprises
- 11:00-11:30 am *Jim Chelikowsky* (UT Austin) - The evolution of Schottky barriers in metal-semiconductor nanofilms
- 11:30am-12:00pm *Kai-Ming Ho* (ISU/Ames Lab) - Coverage Dependent Collective Diffusivity of Dense Pb Wetting Layer on Si(111)

**12:00-1:30 pm Lunch Break**

- Session V Catalysis and Multiscale Modeling** Chair: Bob Helms (UT Dallas)
- 1:30-2:00 pm *Yves Chabal* (UT Dallas) - Molecular Hydrogen dissociation on Ti-doped Aluminum surfaces
- 2:00-2:30 pm *Sok Pantelides* (Vanderbilt U) - Energy issues: Nanocatalysis and battery materials
- 2:30-3:00 pm *Alain Esteve* (Toulouse, France) - Multiscale modelling issues in nanoenergetic materials engineering

**3:00-3:30 pm Coffee Break**

- Session VI Plasmonics & Solar Cells** Chair: Kai-Ming Ho (ISU/Ames Lab)
- 3:30-4:00 pm *Peter Nordlander* (Rice U) - Plasmonic enhancements of light-matter interactions
- 4:00-4:30 pm *Ken Shih* (UT Austin) - Ultra-low Damping of Surface Plasmon Polaritons in Atomically Smooth Epitaxial Ag Films
- 4:30-5:00 pm *Zhenyu Zhang* (U Tennessee) - Quantum tuning of plasmonics for enhanced solar energy conversion
- 5:00-5:30 pm *Efthimios Kaxiras* (Harvard U) - First-principles simulations of hybrid organic-inorganic devices for photovoltaic applications: predictions of efficiency and stability

**6:30 pm Dinner Reception (Hyatt Hotel)**

## Saturday January 22

- Session VII Oxides** Chair: David Langreth (Rutgers U)
- 8:30-9:00 am *Gyula Eres* (ORNL) - Bandgap narrowing of titanium oxide semiconductors by non-compensated anion-cation codoping for enhanced visible-light photoactivity
- 9:00-9:30 am *Norman Mannella* (U Tennessee) - Recent x-ray spectroscopy results in non-compensated doped TiO<sub>2</sub>
- 9:30-10:00 am *Shengbai Zhang* (RPI) - Optimal doping of SiO<sub>2</sub>
- 10:00-10:30 am *Lingzhu Kong* (Princeton U) - Rotational-vibrational frequencies and infrared intensity for van der Waals bonded H<sub>2</sub> in nanoporous materials

**10:30-10:45 am Coffee Break**

- Session VIII Theory & Modeling** Chair: Jim Chelikowsky (UT Austin)
- 10:45-11:15 am *Suhuai Wei* (NREL) - Theoretical study of pseudo-quaternary Cu<sub>2</sub>ZnSn(S,Se)<sub>4</sub> alloy for thinfilm solar cell applications
- 11:15-11:45 am *Qiming Zhang* (UT Arlington) - Amphoteric conductivity of Cu<sub>2</sub>O: first-principles studies
- 11:45am-12:15pm *K.J. Cho* (UT Dallas) - Multiscale design of metal alloy catalysts for clean energy applications

**12:15-12:30 pm Closing Remarks** Kai-Ming Ho & Shengbai Zhang

**12:30-3:00 pm Lunch and CMCSN meeting**