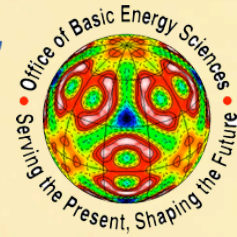




**Office of
Science**

U.S. DEPARTMENT OF ENERGY



**1st ANNUAL COORDINATION MEETING OF THE DOE
COMPUTATIONAL MATERIALS SCIENCE NETWORK (CMSN) on
“PREDICTIVE MODELING OF THE GROWTH AND PROPERTIES OF ENERGY-
RELEVANT THIN FILM AND NANOSTRUCTURES”**

October 31 – November 1, 2008

Location: PARK VISTA HOTEL, GATLINBURG AT SMOKY MOUNTAIN, TENNESSEE

Meeting Coordinators: Kai-Ming Ho & Cai-Zhuang Wang
Zhenyu Zhang

**Ames Laboratory
Oak Ridge National Laboratory**

Program

Room: Mountain View B

Friday, October 31

Opening Session

8:20-8:25 am

Kai-Ming Ho

✦ Opening Remarks

8:25-8:50 am

Malcolm Stocks

✦ Welcome Remarks: The Making of CMSN

Session I 2D Nanostructures

Chair: *Gwo-Ching. Wang*

8:50-9:20 am

Max Lagally

✦ Dancing on Si Nanomembranes

9:20-9:50 am

Ed Conrad

✦ Structure and Growth of Epitaxial Graphene on SiC

9:50-10:10 am

Feng Liu

✦ Predictive Design of Nanomagnetism in Graphene

10:10-10:40 am

Michael Tringides

✦ Forgetting the Main Character: The Leading Role of the Wetting Layer in Growth

10:40-11:10 am Coffee Break

Session II Solar Energy

Chair: *Cai-Zhuang Wang*

11:10-11:40 am

Dan Friedman

✦ Design of III-V Materials for Next-Generation Multijunction Solar Cells

11:40 am-12:10 pm

Judy Wu

✦ Probing Photovoltaic on Single Nanowire Energy Devices

12:10-12:30 pm

Zhenyu Zhang

✦ Tuning Semiconductor Bandgaps via n-p Codoping

12:30-2:00 pm Lunch Break



AMES LABORATORY
United States Department of Energy
Creating Materials and Energy Solutions

Co-Sponsors



Session III Hydrogen Storage

Chair: *Bob Compton*

| | | |
|--------------|-----------------------|--|
| 2:00-2:30 pm | <i>David Langreth</i> | ✦ First-Principles description of Van der Waals Interactions in energy materials |
| 2:30-2:50 pm | <i>Mei-Yin Chou</i> | ✦ Energetics and Kinetics of Metal Hydrides |
| 2:50-3:20 pm | <i>Gwo-Ching Wang</i> | ✦ Mg Nanoblades for Hydrogen Storage |
| 3:20-3:50 pm | <i>Puru Jena</i> | ✦ Nano Materials for Hydrogen Storage |
| 3:50-4:10 pm | <i>Shengbai Zhang</i> | ✦ Weak Interactions in Energy Materials |

4:10-4:40 pm Coffee Break

Session IV Chemical Processes and Catalysis

Chair: *Kai-Ming Ho*

| | | |
|--------------|----------------------|---|
| 4:40-5:10 pm | <i>Wayne Goodman</i> | ✦ Catalysis over Metal Alloys: from Planar Surfaces to Nanoclusters |
| 5:10-5:30 pm | <i>Jim Evans</i> | ✦ Atomistic and Multiscale Modeling of Surface Reactions: From Nanoscale Fluctuations to Mesoscale Reaction |
| 5:30-6:00 pm | <i>Ken Shih</i> | ✦ Adsorbate-induced Nanorestructuring in Quantum Film |
| 6:00-6:30 pm | <i>Pat Thiel</i> | ✦ Chemical Processes on Quasicrystals |

7:00 pm - Dinner reception

Saturday, November 1

Session V 0D and 1D Systems

Chair: *Zhenyu Zhang*

| | | |
|----------------|-----------------------|---|
| 8:30-9:00 am | <i>Ellen Williams</i> | ✦ Interface Dynamics and Electromigration |
| 9:00-9:30 am | <i>Vivek Shenoy</i> | ✦ Compositional Patterning in Strained Nanowires and Quantum Dots |
| 9:30-10:00 am | <i>Boris Yakobson</i> | ✦ New Frontiers of Super-Atoms |
| 10:00-10:20 am | <i>Ted Einstein</i> | ✦ Small Pyramidal Mounds on Cu(001): Role of Impurities in Growth |

10:20-10:40 am Coffee Break

Session VI Films: From Classical to Quantum

Chair: *Ted Einstein*

| | | |
|-------------------|-----------------------|---|
| 10:40-11:10 am | <i>Eric Chason</i> | ✦ Origins of Residual Stress in Thin Films |
| 11:10-11:40 am | <i>Ludwig Bartels</i> | ✦ Surface Dynamics and Pattern Formation |
| 11:40 am-12:10 pm | <i>Tai Chiang</i> | ✦ Complex Electronic Structure in Metal Films - a Pseudogap in Pb |
| 12:10-12:40 pm | <i>Hanno Weiering</i> | ✦ Superconductivity and Plasmonics of Quantum Metal Films and Metallic Alloys |

12:40-2:00 pm Lunch Break

2:00-5:00 pm CMSN discussions and planning