



**ANNUAL COORDINATION MEETING OF THE DOE COMPUTATIONAL  
MATERIALS SCIENCE NETWORK (CMSN) on  
“MULTISCALE STUDIES OF THE FORMATION AND STABILITY OF  
SURFACE-BASED NANOSTRUCTURES”**

**October 14-15, 2005**

**University of Wisconsin-Madison, Madison, Wisconsin**

**Program**

**Friday, October 14—1307 Engineering Research Building**

Chair: K. M. Ho

- 2:00-2:05 pm: M. Lagally – Welcome
- 2:05-2:20 pm: D. Koelling, DOE, CMSN – Program Remarks
- 2:20-2:40 pm: M. Y. Chou – “Quantum Size Effects in Metal Thin Films”
- 2:40-3:00 pm: T. Kaxiras – “Multiscale Simulations for Bulk Solids and Nanostructures”
- 3:00-3:20 pm: C. Z. Wang – “Structures and Diffusion Barriers from ab initio and Tight-Binding Calculations”
- 3:20-3:50 pm: T. C. Chiang – “Quantum Size and Quantum Confinement Effects in Thin Films”
- 3:50-4:20 pm: M. Tringides – “Novel Routes to Self-organization in Metal/Semiconductor Epitaxy”

**4:20-4:50 pm: break, foyer of Research Room, 1025 Engineering Centers Building**

- 4:50-5:20 pm: L. Mawst – “MOCVD Grown Highly Strained Active Regions for Semiconductor Lasers”
- 5:20-5:40 pm: T. Einstein – “Straddling Atomistic/Discrete and Nano/Mesoscale Perspectives on Vicinal Surfaces: Using the Step-Continuum Model to Study the Statistical Mechanics of Steps”
- 5:40-6:00 pm: F. Liu – “Multi-scale Theory and Computation of Strain Engineering and Nanomechanical Architecture of Nanostructures on the Surface”

**7:00 - 9:00 pm: Reception and Buffet Dinner at InnTowner Hotel**

**Saturday, October 15—Research Room, 1025 Engineering Center Building**

Chair: Z. Y. Zhang

9:00-9:30 am: E. Williams –To be announced

9:30-10:00 am: F. Himpsel - “Atomic Wires on Stepped Si Surfaces”

10:00-10:30 am: H. Weiering – “Optimal Doping Control in Dilute Magnetic Semiconductors”

**10:30-11:00 am: coffee break**

11:00-11:20 am: J. Evans – “Modeling Strategies for Multilayer Film Growth: From Atomistic to Step Dynamics to Continuum”

11:20-11:50 am: G. Kellogg – “Spontaneous Self-Assembly of Nanoscale Domain Patterns: Thermodynamics vs. Kinetics”

11:50-12:20 am: D. Schlom – “Enhancing Ferroelectrics Using Strain”

**12:20-2:00 pm: Lunch**

2:00-2:30 pm: P. Evans – “Single-Monolayer Organic Electronics: Structures and Interfaces”

2:30-3:00 pm: M. Lagally – “Silicon-Based Nanomembrane Materials: The Ultimate in Strain Engineering”

**3:00-5:30 pm: coffee & discussions**

5:30 pm: K. M. Ho – Concluding Remarks