

Technical Program

ARO-sponsored Workshop on Atomistic Interfaces 2009 - Ionic Solids (United Technologies Engineering Building room 175, UConn)

Monday Morning (August 24, 2009) – chaired by Hanchen Huang

8:20-8:30	Hanchen Huang	Information
8:30-8:50	Dean Mun Y. Choi	Welcome
8:55-9:25	John Prater Marc Ulrich David Stepp	Opportunities for Research in the Heteroepitaxial and Polycrystalline Growth of Oxide Films and Engineering of Oxide Interface Properties
9:30-10:00	Sidney Yip	Atomistic Studies of Slow Dynamics in Materials Deformation and Flow
10:05-10:20		Coffee Break
10:20-10:50	Pamir Alpay	Interlayer Interactions and Electrical Domain Structures in Compositionally Graded Ferroelectrics
10:55-11:25	Kaushik Bhattacharya	Multiscale Models of Morphotropic Phase Boundaries in multiferroic Perovskites
11:30-12:00	Andrew Rappe	Using Ferroelectric Oxides to Control Surface Chemistry

Monday Afternoon (August 24, 2009) – Chaired by Peter Chung

1:30-2:00	<i>Melanie Cole</i>	<i>Electronic Materials by Design</i>
2:05-2:35	George Gilmer	Simulations of the Sputter Deposition of Be Films Using Kinetic Monte Carlo and Molecular Dynamics Methods: Instabilities that Cause Surface Roughness and Pinholes

2:40-3:10	Eric Chason	Understanding How Competing Kinetic Processes Control Residual Stress Evolution
3:15-3:30		Coffee Break
3:30-4:00	Chang-beom Eom	Way to Realize Magnetoelectric Coupling in Domain Engineered Multiferroic Thin Films
4:05-4:35	Susanne Opalka	Complex Borohydride and H ₂ Interactions with Pt-loaded ZrO ₂ Nanoframeworks
4:40-5:10	Timothy Cale	Grain-Focused Modeling of Thin Film Processing

6:00-7:00: Reception; 7:00-8:30: Dinner at the Nathan Hale Inn

Tuesday Morning (August 25, 2009) – Chaired by Eric Jordan

8:20-8:50	David Vanderbilt	Nonlinear Dielectric Properties of Oxide Interfaces from First Principles
8:55-9:25	Karin Rabe	Epitaxial-strain-induced Ferroelectricity in Oxides
9:30-10:00	Craig Fennie	Design of Multiferroic Materials and Interfaces from First Principles
10:05-10:20		Coffee Break
10:20-10:50	Z. Xiao Guo	Sorption and Binding at Surfaces and Interfaces for Clean Energy
10:55-11:25	Zhenyu Zhang	Predictive Modeling of Interface Modifications for Improved Chemical Functionality
11:30-12:00	Wilson Chiu	Non-Destructive Imaging and Analysis of Electrochemical Reaction Interfaces in a Solid Oxide Fuel Cell

Tuesday Afternoon (August 25, 2009) – Chaired by Moneesh Upmanyu

1:30-2:00	Simon Phillpot	Charge-Optimized Many-Body Potential for Ceramic-Metal and Ceramic-Ceramic Interfaces
2:05-2:35	Peter Chung	MD Simulations of Oxygen Vacancies in BTO
2:40-3:10	Amit Misra	Atomic Scale Design of Interfaces in Nanolayered Composites for High Strengths and High Radiation Damage Tolerance
3:15-3:30		Coffee Break
3:30-4:00	Saroj Nayak	Large Scale Quantum Simulations of Oxide Interfaces
4:05-4:35	Nasr Ghoniem	Atomistic Mechanisms of Twin Boundary Motion in Temperature and Stress Fields
4:40-5:10	Harold Park	Surface Effects on the Elastic Properties and Buckling Stability of Silicon Nanowires

Wednesday Morning (August 26, 2009) – Chaired by Melanie Cole

8:20-8:50	Michael Grinfeld	Stress and Electrostatics Driven Rearrangement Instabilities in Nano- and Macrophysics
8:55-9:25	Fei Gao	Interface Structures for Epitaxial α -Fe ₂ O ₃ on α -Al ₂ O ₃ : TEM Observation and Atomic-level Simulation
9:30-10:00	Hanchen Huang	Surface Characteristic Length Scale During Growth
10:05-10:20		Coffee Break
10:20-12:00	David Stepp Eliot Fang	Panel Discussions: Growth of Ionic Thin Films – Grand Challenges