### CURRICULUM VITAE (06/2008)

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<u>CURRENT POSITION</u>: Professor of Mathematics, Iowa State University
Senior Scientist, Ames Laboratory (U.S. Department of Energy)
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### **CONTACT INFORMATION:**

Ames Laboratory - USDOE, 315 Wilhelm Hall, Iowa State University, Ames Iowa 50011 Telephone: (515)294-1638 Fax: (515)294-0266 Email: evans@ameslab.gov Web page: http://www.external.ameslab.gov/pbchem/PI%20info/evans.htm

### **BIOGRAPHIC INFORMATION:**

Birth date: 2/12/1954. Married to Patricia A. Thiel. Two children: Amanda F. Evans, Ellen R. Thiel.

### **EDUCATION**:

B.Sc. (Honors)	Mathematics	University of Melbourne, Australia	1975
Ph.D.	Mathematical Physics	University of Adelaide, Australia	1979
Postdoctoral Fellow	Chemical Physics	Iowa State University/Ames Laboratory	1979-1982

### PROFESSIONAL EXPERIENCE:

1991-present	Professor (1996-present), Associate Professor (1991-1996),
	Department of Mathematics, Iowa State University (ISU)
1982-present	Senior Scientist (1996-present); Chemist (1993-96), Associate Physicist
-	(1983-93), Assistant Chemist II (1982-83), Ames Laboratory - USDOE
Summer 2000	Visiting Professor, Ecole des Mines & Universite Henri Poincare Nancy I, France
Summer 1991	Visiting Scientist, Fritz Haber Institut der MPG, Berlin, Germany
1989-1991	Adjunct Associate Professor, Department of Mathematics, Iowa State University
1989-1991	Adjunct Associate Professor, Department of Physics, Iowa State University

### **PROFESSIONAL SOCIETIES:**

Society for Industrial and Applied Mathematics (SIAM); American Physical Society (APS); Materials Research Society (MRS); AVS - Science & Technology Society (AVS)

### HONORS:

Fellow, American Physical Society (2002); ISU/LAS Mid-Career Achievement in Research (2005)

### PRIMARY RESEARCH AREA:

*Non-equilibrium Statistical Mechanics* (atomistic lattice-gas models & kinetic Monte Carlo simulation; hybrid, continuum, multiscale treatments) applied to *Modeling of Non-Equilibrium Processes at Surfaces* 

- Growth and relaxation of epitaxial thin films: submonolayer island formation; kinetic roughening; coarsening and sintering; connecting atomistic to continuum treatments; modeling of specific systems
- Spatiotemporal behavior in catalytic surface reactions: reaction kinetics (non-linear dynamics; poisoning transitions); chemical diffusion and front propagation; fluctuations in nanoscale systems
- Complex diffusion and reaction processes on semiconductor surfaces and in mesoporous systems
- Statistical mechanics of fundamental behavior in far-from-equilibrium reaction-diffusion systems

### CURRENT FUNDED RESEARCH PROJECTS AS PI OR CO-PI:

Title: Assembly and Stability of Metal Nanostructures on Surfaces (CHE-0809472) Source of Support: NSF Chemistry Division: Analytical & Surface Chemistry Principle Investigator: J.W. Evans; Co-PI: P.A. Thiel Amount & Period: \$593,000 for 08/08 - 07/10

Title: Spatial Organization in Epitaxial Thin Films and Chemisorbed Layers: Manipulation of Nano- and Meso-scale Structure on Metal Substrates (CHE-0414378)
Source of Support: NSF Chemistry Division: Analytical & Surface Chemistry
Principle Investigator: J.W. Evans; Co-PI: P.A. Thiel
Amount & Period: \$540,000 with \$280,000 for Evans (5 yr total) for 08/01/04 - 07/31/09

Title: Ames Laboratory Chemical Physics Program Source of Support: USDOE Basic Energy Sciences – Chemical Sciences Division Principal Investigators: J.W. Evans and M.S. Gordon Amount & Period: ~\$330,000 with ~\$140,000 for Evans (per annum) for 10/01/07 - 09/30/10

Title: High-Performance Computational Chemistry: Developments in Scalable Electronic Structure Theory, Non-Equilibrium Statistical Mechanics, and Multiscale Modeling
Source of Support: USDOE-BES SciDAC Program in Computational Chemistry
Principal Investigator: M. S. Gordon (PI); Co-PI's: J.W. Evans, K. Ruedenberg, M. Schmidt
Total Award Amount: \$240,000 with \$45,000 for Evans (per annum) for 10/01/06 - 09/30/09

Title: Selective and Efficient Catalysis in 3D Controlled Environments Source of Support: USDOE Basic Energy Sciences, Division of Chemical Sciences PI: V. Linn; Co-PI's: M. Pruski, A. Bakac, A. Saddow, K. Wu, J. Evans, M. Gordon Amount & Period: ~\$600,000 with ~\$15,000 for Evans (per annum) for 10/1/07-09/30/10

Title: Predictive Modeling of the Growth of Energy-Relevant Thin Films and Nanostructures. Source of Support: USDOE-BES Computational Materials Science Network (CMSN) PI's: Z.Zhang, K.-M.Ho (team leaders); Chou, Einstein, Evans, Kaxiras, Liu, Wang, Zhang (task leaders) Amount & Period: \$930,000 (3 year total) for 10/01/08 to 09/30/11

Title: Multiscale Studies of the Formation and Stability of Surface-Based Nanostructures. Source of Support: USDOE-BES Computational Materials Science Network (CMSN) PI's: Z. Zhang, K.-M. Ho (team leaders); Chou, Einstein, Evans, Kaxiras, Shenoy, Wang (task leaders) Amount & Period: \$840,000 with \$50,000 to Evans (3 year totals) for 10/01/04 - 09/30/08

### SUBMITTED PROPOSALS:

Title: A Multi-Scale Approach to addressing Bio-Remediation Source of Support: USDOE GTL/SciDAC Principal Investigators: M. Gordon, T. Windus, M. Lamm, R. Fox, J. Evans Amount & Period: \$1,500,000 (3 year totals) from 10/01/08 to 09/30/11

### PREVIOUS FUNDED NSF PROJECTS AS PI OR CO-PI:

Title/Source: Nanostructure Formation & Evolution in Thin Films (CHE-0078596) NSF Anal/Surf Chem Principal Investigator: J.W. Evans; Co-PI: P.A. Thiel Amount & Period: \$555,969 for August 2000 - July 2005.

Title/Source: Evolution of Thin Film Nanostructures (EEC-0085604) NSF Nano Modeling & Sim - SGI Principal Investigator: T.S. Rahman; Co-PI's: T.L. Einstein, J.W. Evans, K. Fichthorn Amount & Period: for \$1.07 million (with \$228,000 to Evans/ISU) for September 2000 - August 2004.

Title/Source: Growth & Equilibration of Thin Metal Films (CHE-9700592) NSF Analytic/Surface Chem Principal Investigator: J. W. Evans; Co-Principal Investigator: P. A. Thiel.

Amount & Period: \$550,000 (plus \$144,600 in cost-sharing from ISU-IPRT) April 1997 - March 2001.

Title/Source: Nucleation, Growth, Structure of Metal-on-Metal Films (CHE-9317660) NSF Anal/Surf Chem Principal Investigator: J. W. Evans; Co-Principal Investigator: P. A. Thiel. Amount & Period: \$406,000 (plus \$103,000 in cost-sharing from ISU-IPRT). Jan. 1994 – Dec. 1997.

Title/Source: Non-equilibrium Structure of Thin Metal Films (CHE-9014214) NSF Materials Chem Init. Co-Principal Investigators: P. A. Thiel and J. W. Evans

Amount & Period: \$373,000 (plus \$90,000 in matching support from ISU-IPRT). Sept. 1990-Aug. 1994.

Title/Source: REU: Computational Chemistry, Physics, and Mathematics (CHE-0139152) NSF REU Principal Investigator: M.S. Gordon. Co-PI's: J.W. Evans, B. Harmon, K.-M. Ho, et al. Amount & Period: \$144,000 for May 2002 - April 2005.

Title: REU: Computational Chemistry, Physics, and Mathematics (CHE-0453444) NSF REU Principal Investigator: H. Stauffer; Co-PI's: X. Song, M.S. Gordon, J.W. Evans, B. Harmon, et al. Amount & Period: ~\$70,000 for May 2005 - April 2008.

### PREVIOUS FUNDED USDOE-BES PROJECTS AS PI OR CO-PI:

Title: Ames Laboratory Chemical Physics Program, USDOE BES – Chemical Sciences Principal Investigators: J.W. Evans and M.S. Gordon Amount & Period: \$330,000 with \$140,000 for Evans (per annum) for 10/01/04 - 09/30/07

Title: Selective and Efficient Catalysis in 3D Controlled Environments, USDOE - BES Chem. Sci. PI: M. Pruski; Co-PI's: V. Linn, J. Espenson, A. Bakac, R. Angelici, J. Evans, M. Gordon Amount & Period: \$600,000 with \$15,000 for Evans (per annum) for 10/1/03-09/30/07

Title/Source: Modeling of Spatiotemporal Behavior in Surface Reactions, BES - Chemical Sciences Principal Investigator: J. W. Evans

Amount & Period: ~\$120,000 per annum for October 1999 – September 2004

Title/Source: Advancing MR Methods in Electronic Structure Theory. BES SciDAC (Comp Chem) Principal Investigator: M. S. Gordon (PI); Co-PI's: J.W. Evans, K. Ruedenberg Amount & Period: \$240,000 with \$45,000 to Evans (per annum) for 10/01/03 - 09/30/06

Title/Source: Computational Chemistry: Advancing... Electronic Structure Theory. BES SciDAC Principal Investigator: M.S. Gordon; Co-PI's: J.W. Evans and K. Ruedenberg Amount & Period: \$250,000 with ~\$50,000 to Evans (per annum) Oct. 2001 – Sept. 2003

Title/Source: Modeling of Spatiotemporal Behavior in Surface Reactions, BES - Chemical Sciences Principal Investigator: J. W. Evans

Amount & Period: ~\$430,000 total from October 1992 - September 1999

Title/Source: Modeling of Catalytic Surface Reactions in Nanoscale Systems, Ames Lab DOE LDRD Principal Investigator: J. W. Evans Amount & Period: \$26,000 for May - September 1997.

### FUNDED EQUIPMENT PROPOSALS AS CO-PI OR SENIOR COLLABORATOR:

Title: Development of High Performance Low Cost Parallel Computer. Source: NSF MRI PI: Mark Gordon; 4 Co-PI's and several senior collaborators (incl. Evans). Amount & Period: ~\$400,000.

Title: Purchase of Computational Chemistry Hardware. Source: NSF Chemical Instrumentation Program PI: G. Kraus; Co-PI: J. Evans + 5 others; Amount & Period: \$176,000. Oct. 1998 – Sept. 1999.

Title: Purchase of a Parallel Computing Facility. Source: NSF Chemical Instrumentation Program PI: M. S. Gordon; Co-PI: J. Evans + 3 others. Period: \$200,524. Dec. 1993 - May 1995.

Title: Purchase of Graphical Supercomputer. Source: NSF Chemical Instrumentation Program Co-PI's: D. K. Hoffman, J. W. Evans + 3 others. Period: \$197,630. June 1989 - June 1990.

### **RESEARCH IMPACT: CITATION INFORMATION FROM THE ISI WEB OF KNOWLEDGE**

ISI Web of Science: Science Citation Index Expanded (http://isiknowledge.com)

Approximate total number of citations in each year on ISI Web of Science to all published papers with viewable records as of June 2008. **Total Cites: 4,902** for 1979- (including self-cites). **h-index:** 36.

year	93	94	95	96	97	98	99	00	01	02	03	04	05	06	07
cites	152	257	213	276	298	340	292	302	229	268	316	254	261	290	290

Selected highly-cited papers (June 2008 data from ISI including self-cites):

Selected inging cited papers (suite 2000 data noin 151 meruding sen cites).
[11] Evans et al. JCP (1983) Irreversible Random and Cooperative Processes
[21] Nord & Evans, JCP (1985) Irreversible Random Immobile Adsorption
[55] Evans et al., PRB (1990) Low-Temperature Epitaxial Growth181 cites
[60] Evans, PRB (1991) Factors mediating Smoothness in EpitaxialGrowth90 cites
[61] Evans & Miesch, PRL (1991) Kinetics of a First-Order Poisoning Transition
[66] Evans, Langmuir (1991) Kinetic Phase Transitions in Catalytic Reaction Models102 cites
[72] Bartelt & Evans, PRB (1992) Scaling Analysis in Diffusion-mediated Island Growth273 cites
[82] Bartelt & Evans, Surf. Sci. (1993) Nucleation and Growth of Square Islands112 cites
[87] Evans & Bartelt, JVSTA (1994) Nucleation and Growth in Metal Homoepitaxy106 cites
[88] Bartelt & Evans, SSL (1994) Dendritic Islands in Metal-on-Metal Epitaxy50 cites
[91] Gunther et al., PRL (1994) Anisotropy in Nucleation and Growth of 2D Islands
[93] Wen et al., PRL (1994) Diffusion of Large 2D Ag Clusters on Ag(100)197 cites
[96] Tammaro et al., JCP (1995) Hybrid Treatment of Spatiotemporal Behavior inReactions44 cites
[97] Bartelt & Evans, PRL (1995) Transition to Multilayer Kinetic Roughening
[100] Wen et al., PRL (1996) Coarsening Mechanisms in a Metal Film111 cites
[102] Bartelt & Evans, PRB (1996) Exact Island Size Distributions for Deposition
[113] Bartelt et al., PRL (1998) Island Size and Environment Dependence of Adatom Capture46 cites
[114] Stoldt et al., PRL (1998) Evolution of Far-From-Equilibrium Nanostructures
[117] Bartelt et al, PRB (1999) Adatom Capture by Arrays of 2D Islands45 cites
[118] Suchorski et al., PRL (1999) Fluctuation-induced Transitions in a Bistable Reaction
[130] Liu & Evans, PRL (2000) Symmetry-breaking and Percolation in Surface Reaction
[129] Stoldt et al., PRL (2000) Using Temperature to tune Film Roughness
[133] Pai et al., PRL (2001) Evolution of 2D Worm-like Nanoclusters
[140] Caspersen et al. PRB (2002) Development and Ordering of Mounds
[143] Liu & Evans, PRB (2002) Sintering of 2D Nanostructures
[145] Evans & Bartelt, PRB (2002) Island Sizes and Capture Zones: JPD Factorization22 cites
[146] Fournee et al., PRB (2003) Nucleation and Growth on Quasicrystal Surfaces

### CURRENT (C) AND PREVIOUS (P) RESEARCH PROJECTS:

### Morphological Evolution during Growth and Relaxation of Epitaxial Thin Films (funded by NSF):

Development and analysis of models realistically describing the essential physics of growth and relaxation processes in epitaxial thin films. Modeling elucidates experimental observations from scanning tunneling microscopy or surface-sensitive diffraction experiments, often achieving predictive capability. *See Evans, Thiel, and Bartelt, Surface Science Reports, 61, 1-128 (2006).* 

- Submonolayer nucleation and growth of two-dimensional islands during deposition:
  - (i) pioneering simulation studies of island size distributions (ISD) and their scaling behavior (P)
  - (ii) explanation of the failure of mean-field rate equation theories for the ISD and adatom capture (P)
- (iii) special topics: anisotropic systems; transition to reversible island formation; island shape transitions
- (iv) development of beyond-mean-field analytic theories including spatial aspects of nucleation (C)
- (v) development of new coarse-grained simulation algorithms, e.g., Geometry-Based Simulation (C)
- Kinetic roughening and morphological evolution during multilayer film growth:
  (i) explanation of "smooth" growth at low-temperature in terms of "downward funneling" (P)
  (ii) prediction from atomistic models of kinetic roughening for metal(100) homoepitaxy (P)
  (v) analysis of mound formation and evolution, e.g., fluctuation-dominated coarsening (C)
  (vi) development of continuum theories from coarse-grained of step dynamics models (C)
- Predictive modeling of multilayer homoepitaxial growth for specific systems:
  (i) Ag on Ag(100): temperature-dependence; slow mound slope selection; mound coarsening (P)
  (ii) Ag on Ag(111): detailed analysis of "wedding-cake" film morphology (C)
- Post-deposition coarsening processes for submonolayer films:
  (i) diffusion of large 2D clusters experimental discovery and theoretical analysis (P,C)
  (ii) Smoluchowski ripening (cluster diffusion & coalescence) vs. Ostwald ripening (P)
  (iii) shape relaxation during 2D cluster-step & cluster-cluster coalescence, anomalous size scaling (C)
- Complex growth systems: deposition of metal films on quasicrystals rate equation and novel atomistic modeling and KMC of island nucleation; modeling of multilayer growth incl. quantum size effects; film growth on binary alloys quantum size effects; stoichiometric self-growth by co-deposition (C)
- Effect of "chemical additives" on nanostructure evolution in thin metal films (C)

Collaborators include: Patricia Thiel (ISU); Vincent. Fournee (CNRS, Nancy).

### <u>Spatiotemporal Phenomena in Catalytic Surface Reactions (funded by USDOE – Chem. Sciences):</u> Atomistic lattice-gas (LG) modeling provides a fundamental description of reactions such as COoxidation and NO-reduction on metal surfaces, incorporating the influence of ordering and fluctuations in the distribution of adsorbed reactant molecules. These effects are ignored in the traditional mean-field (MF) rate and reaction-diffusion equation formulations. Much of our work has focused on connecting such fundamental atomistic descriptions with meso- or macro-scale kinetics and spatial pattern formation.

• General behavior in non-equilibrium surface reaction models: discontinuous "poisoning" transitions (metastability & nucleation phenomena); non-equilibrium order-disorder transitions & critical phenomena

- Chemical diffusion in mixed adlayers: coverage-dependence, percolation properties, tensorial form (P)
- Connecting-the-length-scales from atomistic ordering to mesoscale pattern formation: we recently developed a Heterogeneous-Coupled-Lattice-Gas (HCLG) simulation approach (C)
- Detailed and realistic atomistic LG models for CO-oxidation on Pd(100) and related reactions (C)
- Fluctuations in surface reactions in nanoscale systems (e.g., on metal field emitter tips): theoretical analysis of noise-induced transitions in bistable systems described by LG rather than MF models (C)

Collaborator: Ronald Imbihl (Universitaet Hannover), Miguel Salmeron (LBNL).

### Modeling of Complex Processes on Si(100) Surfaces (funded by USDOE - SciDAC):

One component of this project is to integrate energetic information from ab-initio quantum chemistry studies into the development of atomistic and coarse-grained models for various complex processes on Si(100) surfaces.

- •Formation of "atomic rows" during deposition of Group III metals on Si(100) (P)
- Morphological evolution during sputtering, and competitive oxidation & etching on vicinal Si(100) (C)

Collaborators: Mark Gordon (ISU)

### **Other Research Projects**:

•Random and Cooperative Sequential Adsorption: irreversible deposition of immobile objects which naturally produces non-trivial, non-equilibrium jammed states. These problems have diverse applications including "space filling" problems of interest in Mathematical Statistics, reactions on polymer chains, colloidal deposition, and chemisorption processes. See J.W. Evans, Rev. Mod. Phys. 75 (1993) 1281.

- Percolation theory and percolative transport
- Non-equilibrium phase transitions & patterns in far-from-equilibrium reaction-diffusion systems
- Heteroepitaxy including quantum size effects and strain (DOE CMSN collaboration with Ho, Wang)
- Transport and reaction in nanoporous systems (DOE Catalysis collaboration with Victor S.-Y. Lin)

### **<u>RESEARCH GROUP MEMBERS</u>**: # = current; (x) = number of co-authored publications

### Professional & Scientific Staff Scientist:

# Dr. Da-Jiang Liu, Assoc. Scientist (36) from 2002-present.Dr. Maozhi Li, Asst. Scientist (12) 2005-2007 (shared with Ames Lab MEP) Asst. Prof. Physics Renmin U.

### Postdoctoral Associates:

# Dr. Yong Han (4) 2007-present (Ph.D Utah 2006)

Dr. Maozhi Li (13) 2001-2005; Asst. Prof. Physics Renmin University, Beijing (Ph.D.CAS-Beijing 2001)
Dr. Chandana Ghosh (4) from 2004-2005. Postdoc, University of Louiville (Ph.D. KSU 2004)
Dr. Da-Jiang Liu (37) from 1998-2001. Staff Scientist: Ames Laboratory/ISU (Ph.D. U Maryland 1998)
Dr. A. M. Cadilhe (4) 1997-1999. Asst. Prof. Physics, U. do Minho, Portugal (Ph.D. Clarkson 1997)
Dr. M. C. Bartelt (23) 1991-1996. Deceased. Formerly Scientific Capability Leader (Director) of the Computational Materials Sci., CMS Lawrence Livermore NL – USDOE (Ph.D. Clarkson 1991)

Dr. H. C. Kang (6) 1990-1991. Assoc. Prof. Chemistry, National U. Singapore (Ph.D. Caltech 1990)

### Ph.D. Students:

# Xiaofang Guo (3) Physics/Applied Math 2004 - present

# David Ackerman, Chemistry 2007 - present

Marvin R. Albao (6) Physics. Graduated Summer 2005. Postdoc FHI-Berlin $\rightarrow$ Nat. Sun Yat-Sen U. Taiwan Kyle J. Caspersen (11) Chemistry. Graduated Fall 2001. Postdoc UCLA/Caltech  $\rightarrow$  Scientist LLNL Edna W. James (4). Math. Grad. Summer 1999. Postdoc Saskatoon/Toronto  $\rightarrow$  Asst. Prof. Math. Algoma U Micheal Tammaro (8). Physics. Graduated Summer 1997. Lecturer, Physics Dept., U. Rhode Island. Timothy R. Ray (2). Mathematics. Graduated Summer 1993. Assoc. Prof. Math., SE Missouri State U.

### M.Sc. Student:

Chris J. Westermeyer. Mathematics. Graduated Spring 1995.

### Graduate Research Assistant:

Changyong Song, Physics (1). Summer 1997.

### NSF REU Undergraduate Trainees (Summer):

Kasey Mathess 2002; Bethany Weinert 2003; Daniel Unruh 2004; Kyle Schnitzenbaumer (3) 2005-6, Kyle Mandsager 2007.

### Ames Laboratory USDOE Undergraduate Research Trainees (Summer):

J. A. Bartz (1) 1986; J. A. Rabaey (1) 1988; M. S. Miesch (2) 1990  $\rightarrow$  Scientist NCAR Boulder; M. Sabella (2) 1992.

### Visiting Scientists:

Miguel Pineda, Spring 2006, Ph.D. student, Chemistry, Universitaet Hannover, Germany Dr. Natalie Pavlenko (2), Fall 2000, Postdoc, Chemistry, Universitaet Hannover, Germany. Prof. Juan Sanchez (1), Summer 1997 & 1998, Physics Dept., U. Mar Del Plata, Argentina. Rainer Dortsch, Summer 1996, Chemistry Diploma student, Universitaet Ulm, Germany.

### **OTHER PERSONNEL** with research projects supervised by JWE (in 1980's):

Ph.D. Students (Chemistry): D. R. Burgess (4); C. K. Chan (3); R. S. Nord (9); D. E. Sanders (7) Postdoctoral Associate: Dr. H. Pak (3)

### TEACHING:

Courses Taught (semester/year: # = number of students: e = evaluation):

Explanation of Evaluation:

Old Scheme: e=1 top 10%; e=2 next 20%; e=3 middle 40%; e=4 next 20%; e=5 bottom 10% \*New Scheme: e=5 excellent; e=4 above average; e=3 average; e=2 below average; e=1 poor

Math 266: Elementary Differential Equations: (F89 #=21 e=2.14) (S90 #=30 e=1.90)

Math 268: Laplace Transforms (S90 #=5 e=1.80)

Chem 563: Statistical Mechanics (S91 #=6 e=1.50)

Math 365: Complex Variables with Applications (S92 #=19 e=1.74)

Math 426: Mathematical Methods for the Physical Sciences (F90 #=24 e=1.25) (F91 #=21 e=1.67) (F92 #=12 e=1.35) (F93 #=21 e=1.67) (F94 #=24 e=1.83) (F95 #=16 e=1.50) (F96 #=18 e=1.33) (F97 #=15 e=1.27) (F98 #=20 e=1.29) (F99 #=15 e=4.80\*) (F00 #=15 e=4.77\*) (F01 #=18 e=4.72\*) (F02 #=13 e=4.62\*) (F03 #=27 e=4.67\*) (F04 #=22 e=4.77\*) (F05 #=12 e=4.50\*) (F06 #=17 e=4.29) (F07 #=20 e=4.29\*)

Math 527: Mathematics of Complex Physical Systems (S93 #=6 e=1.00) (S94 #=6 e=1.33) (S95 #=6 e=1.50) (S96 #=6 e=1.17) (S97 #=6 e=1.43) (S98 #=9 e=1.40) (S99 #=8 e=1.40) (S00 #=7 e=4.71\*) (S01 #=10 e=4.78\*) (S03 #=5 e=5.00\*) (S04 #=9 e=4.67\*) (S05 #=10 e=4.33\*)

Math 646: Mathematical Modeling of Complex Physical Systems (S06 #=7  $e=4.71^*$ ) (S07 #=5  $e=5.00^*$ ) (S08 #=15, e=?)

Special Topics: Math 590 – Synergetics (F91 #=1 e=none); Math 690 W– Probability & Stochastic Processes (S07 #=1, e=none)

Recognition: Outstanding Faculty Instructor for 1992/93: ISU Physics Graduate Student Assoc. Award

### COURSE DEVELOPMENT:

A graduate course, **Math 646: Mathematical Modeling of Complex Physical Systems** (formerly Math 527), was developed to cover the broad spectrum of approaches to modeling of the dynamics of complex physical systems: classical or molecular dynamics; stochastic models and Monte Carlo methods; macroscopic models and non-linear dynamics. This course was designed to meet the interests and key research needs of graduate students in the mathematical, physical, chemical, and materials science disciplines, as well as in certain engineering disciplines. Course material is necessarily drawn from numerous sources, but the presentation is a self-contained, and is accessible to students with various backgrounds. There has been sufficient interest to run the course every year that it has been offered.

### **PUBLICATIONS IN REFEREED JOURNALS**:

- 1. J. W. Evans, "Aspects of the Kinetic Equations for a Special One-dimensional System," J. Austral. Math. Soc. 21 (Series B), 145-175 (1979).
- 2. J. W. Evans, "Velocity Correlation Functions for Finite One-dimensional Systems," Physica 95A, 225-251 (1979).
- 3. J. W. Evans, "The Exact Solution of an Elimination Problem in Kinetic Theory. I. The One-Dimension Hard Sphere Gas," Physica 102A, 87-104 (1980).
- 4. J. W. Evans, "The Exact Solution of an Elimination Problem in Kinetic Theory. II. General Pairwise Interparticle Potentials," Physica 104A, 48-70 (1980).
- 5. J. W. Evans, "The Mathematical Structure of Arrangement Channel Quantum Mechanics," J. Math. Phys. 22, 1672-1686 (1981).
- 6. J. W. Evans and D. K. Hoffman, "Faddeev's Equations in Differential Form: Completeness of Physical and Spurious Solutions and Spectral Properties," J. Math. Phys. 22, 2858-2871 (1981).
- 7. C. K. Chan, J. W. Evans and D. K. Hoffman, "Factorization Relations and Consistency Conditions in the Sudden Approximation," J. Chem. Phys. 75, 722-737 (1981).
- 8. J. W. Evans, D. K. Hoffman and D. J. Kouri, "Scattering Theory in Arrangement Channel Quantum Mechanics," J. Math. Phys. 24, 576-587 (1983)
- 9. J. W. Evans, "Existence and Uniqueness of Bound State Eigenvectors of some Channel Coupling Hamiltonians," J. Math. Phys. 24, 1160-1164 (1983).
- J. W. Evans, D. K. Hoffman and D. J. Kouri, "The Reactive Quantum Boltzmann Equations: A Derivation from an Arrangement Channel Space Representation and BBGKY Hierarchy," J. Chem. Phys. 78, 2665-2681 (1983).
- J. W. Evans, D. R. Burgess and D. K. Hoffman, "Irreversible Random and Cooperative Processes on Lattices: Exact and approximate hierarchy truncation and solution," J. Chem. Phys. 79, 5011-5022 (1983).
- 12. J. W. Evans and D. R. Burgess, "Irreversible Reaction on a Polymer Chain with Range Two Cooperative Effects," J. Chem. Phys. 79, 5023-5028 (1983).
- 13. D. K. Hoffman, J. W. Evans and D. J. Kouri, "The Kinematic Apse and jz-preserving Propensities for Nonreactive, Dissociative, and Reactive Polyatomic Collisions," J. Chem. Phys. 80, 144-148 (1984).
- 14. J. W. Evans, D. K. Hoffman and D. R. Burgess, "Competing Irreversible Cooperative Reactions on Polymer Chains," J. Chem. Phys. 80, 936-943 (1984).
- 15. J. W. Evans, "Irreversible Random and Cooperative Processes on Lattices: Direct Determination of Density Expansions," Physica 123A, 297-318 (1984).
- 16. J. W. Evans and D. K. Hoffman, "Exact Kinetics for 'Almost Random' Irreversible Filling of Lattices," J. Stat. Phys. 36, 65-80 (1984).
- 17. N. O. Wolf, J. W. Evans and D. K. Hoffman, "Exactly Solvable Irreversible Filling of Lattices," J. Stat. Phys. 36, 2519-2526 (1984).
- J. W. Evans, "Exactly Solvable Irreversible Processes on Bethe Lattices," J. Math. Phys. 25, 2527-2532 (1984).
- 19. J. W. Evans, D. K. Hoffman, "Dynamics of Two-Point Spatial Correlations for Randomly Hopping Lattice Gases: One-Dimensional Models," Phys. Rev. B 30, 2704-2714 (1984).
- 20. J. W. Evans, D. R. Burgess and D. K. Hoffman, "Irreversible Random and Cooperative Processes on Lattices: Spatial Correlations," J. Math. Phys. 25, 3051-3063 (1984).

- 21. R. S. Nord and J. W. Evans, "Irreversible Immobile Random Adsorption of Dimers, Trimers, ... on 2D Lattices," J. Chem. Phys. 82, 2795-2810 (1985).
- 22. J. W. Evans and R. S. Nord, "Random Dimer Filling of Lattices: 3D Application to Free Radical Recombination Kinetics," J. Stat. Phys. 38, 681-705 (1985).
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- 183. Y. Han, J.W. Evans, and D.-J. Liu, "Quantum Stabilities and Growth Modes of Thin Metal Films: Unsupported and NiAl-supported Ag Films", Surface Science, in press (2008).

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- 187. M. Albao, F.-C. Chuang, and J.W. Evans, "Kinetic Monte Carlo simulation atomistic models for oxide island formation and step pinning during etching by oxygen of vicinal Si(100)", Thin Solid Films, submitted (2008).
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- 189. D.-J. Liu and J.W. Evans, "Atomistic and multiscale modeling of CO-oxidation on Pd(100) and Rh(100): From nanoscale fluctuations to mesoscale reaction fronts", Surf. Sci. (Invited for Ertl Issue), submitted (2008).
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### **TO BE SUBMITTED:**

- 193. D. Zorn, M. Albao, J.W. Evans, and M.S. Gordon, "Binding and diffusion of Al adatoms and dimers on the Si(100)-2x1 surface: A hybrid QM/MM embedded cluster study", to be submitted.
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- 196. Baris Unal, V. Fournee, P.A. Thiel, and J.W. Evans, "Growth of Height-Selected Ag Islands on 5-fold i-AlPdMn Quasicrystalline Surfaces: STM Analysis and Step Dynamics Modeling", to PRL

### **INVITED PUBLICATIONS IN TOPICAL RESEARCH VOLUMES:**

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- 12. Da-Jiang Liu, Cheol Ho Choi, Mark S. Gordon, and J.W. Evans, "Modeling of the Transition from Active to Passive Oxidation of Si(100)", ibid, MRS Proceedings 619 (MRS, Pittsburgh, 2000), pp.173-178.

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- 13. C.R. Stoldt, K.J. Caspersen, M.C. Bartelt, C.J. Jenks, J.W. Evans, and P.A. Thiel, "Kinetic Roughening of Multilayer Ag/Ag(1000) Films: Complex Temperature Dependence in a Simple System", ibid, MRS Proceedings 619 (MRS, Pittsburgh, 2000), pp. 15-25.
- Da-Jiang Liu, C.R. Stoldt, P.A. Thiel, and J.W. Evans, "Sintering of Metal(100) Homoepitaxial Islands: Kink Rounding Barriers, Modified Size Scaling, and Experimental Behavior", MRS Proceedings 749 on "Morphological and Compositional Evolution of Thin Films", edited by M.J. Aziz, N.C. Bartelt, I. Berbezier, J.B. Hannon, & S.J. Hearne (MRS, Pittsburgh, 2003), W.2.8.1-6.
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- 16. Maozhi Li, M.C. Bartelt, and J.W. Evans, "Beyond-mean-field treatments of island formation during submonolayer deposition: island size distributions for large critical sizes", MRS Proceedings 859E on "Modeling of Morphological Evolution at Surface and Interfaces", edited by J.W. Evans, C. Orme, M. Asta, and Z. Zhang (MRS Pittsburgh, 2005), JJ.3.1.1-6.
- 17. A.R. Layson, K.J. Caspersen, C.R. Stoldt, P.A. Thiel, and J.W. Evans, "Mound formation and evolution during Ag/Ag(100) homoepitaxy: analysis of ultra-rough growth in a prototypical smooth growth system", MRS Proceedings 859E on "Modeling of Morphological Evolution at Surface and Interfaces", edited by J.W. Evans, C. Orme, M. Asta, and Z. Zhang (MRS Pittsburgh, 2005), JJ3.3.1-6.
- M.A. Albao, D.-J. Liu, C.H. Choi, M.S. Gordon, and J.W. Evans, "Competitive etching and oxidation of vicinal Si(100) surfaces", MRS Proceedings 859E on "Modeling of Morphological Evolution at Surface and Interfaces", edited by J.W. Evans, C. Orme, M. Asta, and Z. Zhang (MRS Pittsburgh, 2005), JJ3.6.1-6.

### **INVITED SEMINARS AT OTHER INSTITUTIONS AND INVITED CONFERENCE TALKS:**

### 2008:

"Predicting Multilayer Growth Morphologies of Ag Films controlled by Step Edge Barriers and Quantum Size Effects", American Society of Crystal Growth West Meeting, Fallen Leaf Lake, S. Lake Tahoe, CA June 2008.

"Coarsening of Island Distributions on Surfaces: Ostwald vs Smoluchowski vs Anomalous Ripening", SIAM Conference on "Mathematical Aspects of Materials Science", Minisymposium: Clustering, Coagulation and Coarsening Dynamics Philadelphia May 2008.

"Step dynamics modeling of multilayer growth: Step edge barriers, quantum size effects, & fluctuations" SIAM Conference on "Mathematical Aspects of Materials Science", Minisymposium: Kinetics and Fluctuations of Crystal Surfaces: From Discrete Models to Continuum, Philadelphia May 2008.

"Predicting Multilayer Growth Morphologies of Ag Films controlled by Step Edge Barriers and Quantum Size Effects", Workshop on "Facets of Heteroepitaxy: Theory, Experiment, and Computation", Banff International Research Station, Banff, Alberta, Canada, Feb. 2008

### **2007**:

"Growth of Ag films on Alloy Substrates", CMSN Coordinating Meeting, Iowa State U., Ames, Oct 2007

"Kinetic Monte Carlo Simulation of Epitaxial Thin Film Growth" 13<sup>th</sup> Int. Summer School on Crystal Growth, Park City, Utah, August 2007.

"Kinetic Monte Carlo Simulation of Epitaxial Thin Film Growth", Department of Materials Science, U. Utah, August 2007.

### **2006**:

"Metal film growth on complex substrates: 5-fold surfaces of icosohedral quasicrystals", CMSN Coordinating Meeting, U. Maryland – College Park, October 2006.

"Morphological evolution in thin film homoepitaxy: Modeling and experimental studies of unstable multilayer growth" Inst. Materials Research, Tohoku University, Sendai, Japan, June 2006.

"Simultaneous etching and oxidation of vicinal Si(100): Modeling the evolution of complex step morphologies", Center for Interdisciplinary Research, Tohoku University, Sendai, Japan, June 2006.

"Morphological evolution in thin film homoepitaxy: Modeling and experimental studies of unstable multilayer growth" Inst. Solid State Physics, University of Tokyo, Kashiwa, Japan, June 2006.

### **INVITED SEMINARS AT OTHER INSTITUTIONS AND INVITED CONFERENCE TALKS:**

### 2005:

"Atomistic Modeling of Cooperative Phenomena in Surface Reaction Processes", USDOE BES Meeting on Condensed Phase and Interfacial Molecular Science, Arlie House, Warrenton, VA, October 2005.

"Atomistic Modeling of Cooperative Phenomena in Surface Reactions", Lawrence Berkeley National Laboratory, Berkeley, October 2005.

"Modeling Strategies for Unstable Multilayer Growth: From Atomistic to 2D Continuum Step Dynamics to 3D Continuum", CMSN Coordinating Meeting, U. Wisconsin – Madison, October 2005.

"From Atomic Scale Ordering to Mesoscale Reaction Front Propagation: Analysis of Bistable Surface Reactions", Workshop on "Multiscale Modeling in Condensed Matter and Materials Sciences", Inst. For Pure & Applied Mathematics, UCLA, October 2005.

"Integrated Modeling and Experimental Studies of Homoepitaxial Thin Film Growth", APS Workshop on Surface and Interface Science, Argonne National Laboratory, September 2005.

"From Atomic Scale Ordering to Mesoscale Pattern Formation in Surface Reactions: HCLG Simulation Approach", Inst. Math. Applic. Atomistic Motion to Macroscale Models Workshop, U. Minn, April. 2005

"Atomistic and Continuum Modeling Strategies for Homoepitaxial Thin Film Growth", Institute of Mathematics & Applications, University of Minnesota, Feb. 2005

"Atomistic Models for Low-Temperature Growth of Epitaxial Metal Films" at the workshop on "The Physics of Ultra-thin Films near the Metal-Insulator Transition II", at Brookhaven National Laboratory, January 2005 (trip cancelled due to weather; powerpoint presentations sent instead)

"From Atomic Scale Ordering to Mesocale Reaction Front Propagation: CO-oxidation on Pd(100)", Department of Chemistry, National University of Singapore, January 2005

"Atomistic and Continuum Modeling of Homoepitaxial Thin Film Growth", at the workshop on "Nanoscale Material Interfaces: Experiment, Theory, and Simulation", Institute for Mathematical Sciences, National University of Singapore, January 2005.

### 2004:

"Formation and Relaxation of Submonolayer Films: Atomistic and Continuum Modeling Approaches", CNRS UJF – Grenoble, France, Sept. 2004

"From Atomic Scale Ordering to Mesoscale Front Propagation: HCLG Simulations for CO-oxidation on Pd(100)", CECAM Workshop on "Dynamics at the Mesoscale", Lyon, France, Sept. 2004

"Coarsening Processes in Homoepitaxial Thin Films: Atomistic and Continuum Modeling", SIAM Conference on Mathematical Aspects of Materials Science, Los Angeles, May 2004.

"Predictive Models for Nanostructure Evolution during Epitaxial Thin Film Growth", March Meeting of the American Physical Society, Monteal, March 2004.

### **INVITED SEMINARS AT OTHER INSTITUTIONS AND INVITED CONFERENCE TALKS:**

### 2003:

"Atomistic and Continuum Modeling of Thin Film Growth and Relaxation" CMSN Proposal Formulation Workshop, Emory University, Atlanta, GA Jan. 2003

"Fluctuations and Patterns in Surface Reactions: A Statistical Physics Approach" Conference on Catalysis, Chalmers University, Goteburg, Sweden March 2003.

"Comparison of homoepitaxial film growth for Ag/Ag(100) and Ag/Ag(111)", Kansas State University, Manhattan, Kansas, May 2003.

"Predictive Models of Epitaxial Thin Film Growth: Atomistic and Continuum Approaches" Workshop on "Nonequilibrium Interface Dynamics: Theory and Simulation from Atomistic to Continuum Scales" Center for Scientific Computation and Mathematical Modeling, U. Maryland, Oct. 2003

### 2002:

"Growth & Relaxation of Epitaxial Thin Films: Atomistic & Continuum Modeling", Plenary Talk UCLA Inst. Pure Applied Math Workshop "Math. in Nanoscale Science", Lake Arrowhead, Ca, Dec 2002.

"Multilayer Growth of Metal Homoepitaxial Films: Formation and Evolution of Mounds", Ecole des Mines, Nancy, France, June 2002.

"Nanostructure Formation and Relaxation in Metal(100) Homoepitaxial Systems", Institute of Surface Physics, Universitaet Hannover, Hannover, Germany, June 2002.

"Fluctuations and Reaction Fronts in a Lattice-Gas Model for CO-Oxidation", Department of Physics, Humboldt Universitaet, Berlin, Germany, June 2002.

"Fluctuations and Reaction Fronts in a Lattice-Gas Model for CO-Oxidation", Conference on "Fronts, Fluctuations, and Growth", Michigan Center for Theoretical Physics, U Michigan, Ann Arbor, May 2002.

"Interacting Particles Systems Models for Surface Adsorption and Reaction", Department of Mathematics, Monash University, Australia, May 2002.

"Formation and Evolution of Mounds during Ag/Ag(100) Growth", Int. Seminar on "Models of Epitaxial Crystal Growth", Max Planck Inst. fur Physik Complexer Systeme, Dresden, Germany, Mar 2002.

"Nanostructure Evolution in Thin Film Growth and Relaxation", Department of Physics, Kansas State University, Manhattan, Kansas, February 2002.

### **2001**:

"Growth and Relaxation in Submonolayer Epitaxial Films", 26th International Nathiagali Summer College on Physics and Contemporary Needs (INSC), Nathiagali, Pakistan, July 2001.

"Multilayer growth of Epitaxial Films: Kinetic Roughening and Mound Formation", 26th INSC, Nathiagali, Pakistan, July 2001.

"Nanostructure Evolution in Submonolayer Films", 26th INSC, Nathiagali, Pakistan, July 2001.

"Non-linear Dynamics, Pattern Formation, and Fluctuations in Atomistic Models for Surface Reactions", 26th INSC, Nathiagali, Pakistan, July 2001.

"Multilayer Growth in Metal(100) Homoepitaxy: Key processes in Predictive Atomistic Models", NATO Advanced Research Workshop, Corfu, Greece, June 2001.

"Nanostructure Formation and Relaxation in Metal(100) Homoepitaxial Systems", Kamerlingh-Onnes Laboratory, University of Leiden, The Netherlands, June 2001.

"Nanostructure Formation and Relaxation in Metal(100) Homoepitaxial Systems", Department of Applied Physics, University of Twente, The Netherlands, June 2001.

### **INVITED SEMINARS AT OTHER INSTITUTIONS AND INVITED CONFERENCE TALKS:**

### 2000:

"Morphological Evolution during Multilayer Growth of Metal Films", for "Computer Simulation in Electrochemistry" Symposium, 220th National ACS Meeting, Washington DC, August 2000.

"Simulations of Submonolayer Epitaxy and Etching", ibid , Washington DC, August 2000.

"Growth and Relaxation of Thin Metal Films", Physics, University of Maryland, August 2000.

"Temperature Dependence of Epitaxial Growth in Metal Films: Surprising Behavior in Simple Systems", CECAM Workshop on "Growth, Morphology, and Magnetic Properties of Epitaxial Metallic Systems", Lyon, France, July 2000.

"Developments in Submonolayer Growth and Relaxation of Homoepitaxial Metal Films", Dipartimento di Fisica, Universita degli Studi di Firenze, Florence, Italy, July 2000.

"Ordering, Percolation, and Diffusion in Atomistic Models for Surface Reactions", CECAM Workshop on "Catalysis from First-Principles", Lyon, France, July 2000.

"Chemical Wave Propagation in Lattice-Gas Models of Surface Reactions: Analysis of the Hydrodynamic Limit", CECAM Workshop on "Statistical and Dynamical Aspects of Surface Reactions: Theory, Modeling, and Experiments", Lyon, France, July 2000.

"Temperature-Dependence of Multilayer Growth of Ag/Ag(100)", Department of Physical Chemistry, Universitaet Ulm, Germany, June 2000.

"Interplay between Ordering, Percolation, and Transport in Disordered Systems", Laboratoire de Science et Genie des Materiaux Metalliques (CNRS), Ecole des Mines, Nancy, France, June2000.

"Multilayer Growth of Ag/Ag(100) Homoepitaxial Thin Films", Bonassola workshop on Nanoscale Modification of Surfaces and Thin Films, Bonassola, Italy, May 2000.

### **1999**:

"Homoepitaxial Growth at Low Temperatures: Some Surprises for Simple Systems", DOE supported Workshop on "The Physics of Ultrathin Films near the Metal-Insulator Transition", Brown University, RI, December 1999.

"Non-Equilibrium Growth and Post-Deposition Relaxation of Epitaxial Thin Films", Physics Colloquium, University of Rhode Island, December 1999.

"Spatio-Temporal Behavior in Surface Reactions: Chemical Diffusion, Chemical Waves, and Fluctuations", Sandia National Laboratories, Livermore, California, February 1999.

"Growth and Relaxation of Epitaxial Metal Thin Films", Materials Research Laboratory, University of Illinios, Urbana-Champaign, Illinios, January 1999.

### **INVITED SEMINARS AT OTHER INSTITUTIONS AND INVITED CONFERENCE TALKS:**

### **1998**:

"Formation and Relaxation of Two-Dimensional Metal Islands on Surfaces", Fall MRS Symposium on "Surface and Interface Structure and Dynamics", Boston, December, 1998.

"Formation and Relaxation of Island Distributions in Metal Epitaxy", Workshop on "Bridging the Time and Length Scales in Modeling Epitaxial Growth". NSF/DARPA project on "Virtual Integrated Prototyping (VIP) for Epitaxial Growth", Hughes Research Labs, Malibu, California, August 1998.

"Chemical Diffusion and Wave Propagation in Surface Reactions", Abteilung Physical Chemie, Fritz-Haber-Institute, Berlin, Germany, June 1998.

"Formation and Relaxation of 2D Island Distributions in Metal Epitaxy", 19th International Seminar on Surface Physics, Polanica Zdroj, Poland, June 1998.

"Growth and Relaxation of Metal Epitaxial Films: Ag/Ag(100)", Abteilung Theorie, Fritz-Haber-Institute, Berlin, Germany, June 1998.

"Chemical Diffusion and Wave Propagation in Lattice-Gas Models of Surface Reactions", Workshop on "Recent Advances in Computer Simulation Studies in Condensed Matter Physics", Center for Simulational Physics, University of Georgia, Athens, Georgia, February 1998.

#### **1997**:

"Formation of Islands and Mounds during Epitaxial Growth of Metal Films", Joint US-Argentina Workshop on "Structure and Topography of Surfaces", La Plata, Argentina, November 1997.

"Chemical Diffusion and Wave Propagation in Catalytic Surface Reactions", Joint US-Argentina Workshop on "Structure and Topography of Surfaces", La Plata, Argentina, November 1997.

"Formation of Islands and Mounds during Metal(100) Homoepitaxy", 15th Conf. on Crystal Growth and Epitaxy (Amer. Assoc. Crystal Growth - West), Fallen Leaf Lake, California, June 1997.

"Kinetic Roughening and Mounding during Metal(100) Homoepitaxy", J. W. Evans and M. C. Bartelt, Spring Meeting of the Japanese Physical Society, Symposium on "Dynamical Processes during Epitaxial Growth", Nagoya, Japan, March, 1997.

"Post-deposition Dynamics of Metal(100) Homoepitaxial Adlayers: Cluster Diffusion, Restructuring, and Coarsening", US-Japan Seminar on "Surface Dynamics and Structures during Epitaxial Growth", Nagoya, Japan, March 1997.

"Kinetic Phase Transition during Metal(100) Homoepitaxy between Temperature Regimes of Smooth Growth and Mounding", J. W. Evans and M. C. Bartelt, US-Japan Seminar on "Surface Dynamics and Structures during Epitaxial Growth", Nagoya, Japan, March 1997.

### **INVITED SEMINARS AT OTHER INSTITUTIONS AND INVITED CONFERENCE TALKS**: 1996.

### 1996:

"Growth and Equilibration of Metal(100) Homoepitaxial Films", Physics Department, University of Michigan, Ann Arbor, Michigan, September, 1996.

"Submonolayer Nucleation and Growth, and the Transition to Multilayer Kinetic Roughening during Metal(100) Homoepitaxy", NATO ASI on "Surface Diffusion", Rhodes, Greece, August, 1996.

"Growth and Equilibration of Metal Homoepitaxial Films", Institut de Physique Experimentale, EPF Lausanne, Lausanne, Switzerland, July, 1996.

"Non-linear Diffusion and Chemical Wave Propagation in Surface Reactions", CECAM Workshop on "Pattern Formation in Surface Reactions", Lyon, France, June, 1996.

"Microscopic Models of Spatiotemporal Behavior in Surface Reaction", ESF Workshop on "Surface Restructuring & Non-Linear Dynamics in Reactions at Metal Surfaces", Cambridge, England, Jan. 1996.

### **1995**:

"Modeling of Wave Propagation and Explosions in Surface Reactions", European Science Fdn. Workshop: "Adsorption & Catalytic Reaction Dynamics at Surfaces", Monterosso, Italy, Dec., 1995.

"Transition to Multilayer Kinetic Roughening", Gordon Research Conference on "Epitaxial Thin Films and Interfaces", New Hampshire, July 1995.

"From Submonolayer to Multilayer Growth in Metal (100) Homoepitaxy", Institüt für Oberflächen Chemie, Universitat, Ulm, Germany, May 1995.

"Diffraction Studies of Kinetically Roughening Epitaxial Films", Institüt für Festkörperphysik, Universität, Hannover, Germany, May 1995.

"Transition from Submonolayer Growth to Multilayer Kinetic Roughening: Metal(100) Homoepitaxy", WE-Hereaus Seminar: "Continuum & Atomistic Aspects of Morphological Features of Crystalline Surfaces /Small Particles," Bad Honnef, Germany, May 1995.

"Epitaxial Thin Film Growth", Dept. of Physics, Univ. of Missouri at Columbia, March 1995.

"Nucleation, Growth, and Kinetic Roughening of Epitaxial Thin Films," WE-Hereaus Seminar on "Fundamentals of Epitaxial Growth," Physikzentrum Bad Honnef, Germany, February 1995.

"Random and Cooperative Sequential Adsorption: Models for Chemisorption, Surface Reaction and Epitaxial Growth," (90 min) Les Houches School on "Space Filling Problems," France, Jan. 1995.

### **1994**:

"Nucleation, Growth, and Kinetic Roughening of Metal-on-Metal Epitaxial Thin Films," J. W. Evans and M. C. Bartelt, Fall Meeting of the Materials Research Society, Boston, Dec. 1994.

"Far-From-Equilibrium Surface Adsorption and Reaction Processes", Department of Chemistry and Laboratory for Surface Studies, University of Wisconsin-Milwaukee, October 1994.

"Nucleation, Growth, and Roughening of Thin Films," Plenary Lecture for Symposium on "Experiments and Simulations of Surface Processes", San Luis, Argentina, August 1994.

"Mean-Field versus Lattice-Gas Models for Surface Reactions: Interface Propagation and Nucleation Phenomena", lead talk at ESF Workshop on "Adsorption & Catalytic Reaction Dynamics at Surfaces," Cambridge University, Cambridge, England, April 1994.

"Hybrid Models for Spatiotemporal Behavior in Surface reactions", ibid, Cambridge, April 1994.

A Lattice-Gas Model mimicking the NO + CO Reaction in Pt(100), ibid, Cambridge, April 1994.

"Far-From-Equilibrium Processes at Surfaces," Physics Dept., Georgia Tech., Atlanta, Feb. 1994.

### **INVITED SEMINARS AT OTHER INSTITUTIONS AND INVITED CONFERENCE TALKS:**

### **1993 AND EARLIER:**

"Nucleation and Growth in Metal-on-Metal Homoepitaxy: Rate Equations, Simulations and Experiments," 40th Nat. Symposium AVS, Orlando, November 1993.

"Nucleation and Growth in Metal-on-Metal Homoepitaxy," NIST, Gaithersburg MD, October 1993.

"Nucleation and Growth in Metal-on-FCC(100) Metal Epitaxy," Abteilung fur Oberflächenchemie and Katalyse, Universität Ulm, Ulm, Germany, June 1993.

"Simple Lattice-Gas Model for the NO + CO Reaction on Pt(100)," CECAM Workshop: Random Sequential Addition and Generalizations, Orsay-France, June 1993

"Spatial Correlations for Cooperative Sequential Adsorption with Clustering and Limiting Continuum Processes," *ibid*, Orsay, France, June 1993.

"Irreversible Island Formation during Deposition: Size & Separation Distributions; Diffraction Profiles," U.S.-Japan Seminar on Surface Characterization, Hawaii, March 1993.

"Scaling of Roughness & Bragg-Oscillation Decay during Low-Temperature Epitaxial Growth," ibid 1993.

"Modeling Surface Adsorption and Reaction Processes," Chemical Engineering Dept., Purdue, Jan. 1993.

"Spatio-Temporal Behavior in Surface Reactions: Mean-Field versus Lattice-Gas Modelling," Physics Department, Clarkson University, Potsdam, December 1992.

"Irreversible Island Formation in Surface Deposition Processes: Island Size and Separation Distributions," Institute für Festkörperphysik, Universität Hannover, Hannover, August 1992.

"Comparison of Mean-Field, Lattice-Gas, and Hybrid Models of Surface Reaction", Fritz-Haber-Institute der Max-Plank-Gessellschaft, Berlin, August, 1992.

"Far-From-Equilibrium Thin-Film Growth Processes," DRECAM/SRSIM Division; Commissariat a L'Energie Atomique Saclay, Gif-sur-Yvette, France, July 1992.

"Surface Roughness and Bragg Oscillation Decay in Low-Temperature Epitaxial growth," CECAM Discussion Meeting on Applic. of Random Sequential Adsorption Process, Orsay, France, July 1992.

"Applications of Random & Cooperative Sequential Adsorption to Chemisorption Processes," ibid 1992.

"Kinetic Phase Transitions in Surface Reactions," Dept. Chem. Engineering, U. Minnesota, April 1992.

"Kinetic Phase Diagrams for Catalytic Surface Reactions," Department of Chemical Engineering, University of California, Santa Barbara, March 1992.

"Stochastic Models for Surface Adsorption," Dept. of Statistics, University of Iowa, November 1991.

"Modeling of Epitaxial Thin-Film Growth at Low-Temperature," Institute für Festkörperphysik, Universität Hannover, Hannover, August 1991.

"Bistability versus Discontinuous Transitions in Lattice Models of Catalytic Reactions," Fritz-Haber-Institute der Max-Planck-Gesellschaft, Berlin, August 1991.

"Modeling of Epitaxial Thin-Film Growth at Low-Temperature," Institute für Festkörperforschung, Forschungzentrum KFA, Jülich, July 1991.

"Kinetic Phase Transition, Catalytic Reactions, and Epidemics," Institute für Theoretische Physik der Universität zu Köln, Köln, July 1991.

"Characterization of Non-Equilibrium Micro-Structure," Dept. of Physics U. Auckland, NZ Aug. 1988.

"Non-Hermitian Hamiltonians in Arrangement Channel Quantum Mechanics," Chem., UBC, Feb. 1983.

"On the Solution to Faddeev's Equations in Differential Form, Workshop on Few Body Problems, Brown University, August 1979

### <u>CONTRIBUTED CONFERENCE TALKS (T) AND POSTERS (P), AND DEPARTMENT</u> <u>SEMINARS OR COLLOQUIA AT IOWA STATE UNIVERSITY (S)</u>:

(T) "Kinetics of Facile Bilayer Island Formation for Ag on NiAl(110)" March APS Meeting, New Orleans 2008.

(T) "Modeling of Coarsening in Thin Films: Ostwald vs. Smoluchowski vs. Anomalous Coarsening", CAM Seminar ISU Math, Mar. 2008.

(P) "Complex Wedding-Cake Morphologies in Ag/Ag(111) Film Growth: Predictive Analysis from Realistic Atomistic Modeling", BIRS Workshop on Heteroepitaxy, Banff, Canada Feb. 2008

(T) "Evolution of Complex Morphologies in Homoepitaxial Thin Film Growth: Integration of STM Experiments and Predictive Atomistic Modeling", Condensed Matter Physics Seminar, ISU, September 2007.

(T) "Atomistic and Coarse-Grained Continuum Modeling of Reaction Processes", CAM Seminar ISU Math, 2007.

(T) "Realistic Modeling of Complex Physical and Chemical Systems", Grad Student Colloq., ISU Math, Fall 2007.

(T) "Far-From-Equilibrium Surface Reaction Processes", Ames Lab, Chem Physics on-site review, April 2007.

(T) "Modeling of Polymerization in Mesoporous Silica", Ames Lab, Catalysis on-site review, April 2007.

(T) "Exploring Complex "Wedding-Cake" Film Morphologies: Ag/Ag(111)", AVS, San Fransisco, Nov, 2006.

(T) "Mathematical Modeling of Complex Systems", Graduate Student Colloquium, ISU Math, Fall 2006.

(T) "Step dynamics modeling of mound slope and shape selection", APS, Baltimore, Mar. 2006.

(P) "Al Thin Film Growth on Al-rich 5f Quasicrystals", 9th Int. QC Conf., ISU, Ames IA May 2005

(P) "Atomistic & Continuum Modeling of Thin Film Growth", IMA, U. Minn. MN, April 2005

(T) "Growth & Equilibration of Epitaxial Metal Films: Modeling & Expt", ISU MSE Dept Colloqu.., March 2005.

(T) "Atomistic and Continuum Modeling of Epitaxial Thin Film Growth", CAM Seminar, ISU Math Dept. Jan 2005

(T) "Applied Math meets Materials Science: Modeling of Thin Film Systems", ISU Student Math Club, 2004

(P) "Mound Formation and Evolution in Ag/Ag(100) Homoepitaxy", Fall MRS, Boston, Dec. 2004.

(T) "Far-From-Equilibrium Surface Reaction Processes", Ames Lab, Chem Physics on-site review, April 2004.

(T) "KMC, Hybrid, Multiscale Simulation Approaches to Surface...", Ames Lab Sci-DAC Review, Apr 2004

(T) "Geometry-based Simulation of Submonolayer Film Growth" 50th AVS, Baltimore, MD Nov. 2003

(T) "Atomistic and Continuum Modeling of Thin Film Growth & Relaxation", CAM Seminar, ISU Math 2003

(T) "Beyond-Mean-Field Rate Equn Theories for Island Nucleation & Growth", APS, Austin, Mar. 2003

(P) "Advances in Computational Chemistry @ Ames Lab" USDOE SciDAC Mtg, Napa, CA, March 2003

(S) "Overview of Nucleation and Growth on Surfaces", Ames Lab Materials & Eng. Physics Feb. 2003

(T) "Island Sizes and Capture Zone Areas in Submonolayer Deposition", Fall MRS, Boston, Dec. 2002.

(T) "Kinetic Roughening & Mound Evolution during Ag/Ag(100) Homoepitaxy:", EMRS, Strasbourgh, June 2002.

(P) "Sintering of 2D Nanoclusters in Metal(100) Homoepitaxial Systems", ibid, France, June 2002.

(P) "Kinetic Roughening...for Ag/Ag(100)", "Fronts, Fluctuations, Growth" Conf. @ MCTP U Mich, May 2002.

(P) "Sintering of 2D Nanoclusters on Metal(100) Surfaces", ibid, U Michigan, May 2002.

(T) "Atomistic Modeling of Mound Evolution: Ag/Ag(100) Homoepitaxy", Fall MRS, Boston, Dec 2001.

(S) "Mathematical Modeling of Nanostructure Evolution in Thin Films", ISU Math Dept, Spring, 2001.

(T) "Predictions of Island Nucleation: Etch Pits on Si(100)", March APS, Minneapolis, March 2000.

### <u>CONTRIBUTED CONFERENCE TALKS (T) AND POSTERS (P), AND DEPARTMENT</u> <u>SEMINARS OR COLLOQUIA AT IOWA STATE UNIVERSITY (S)</u>:

(T) "Percolative Diffusion....Influence on Chemical Wave Propagation", 218th Nat. ACS, New Orleans, Aug 1999.

(S) "Spatiotemporal Behavior in Catalytic Surface Reactions", Ames Lab Chem. Sci. Review, May, 1999.

(T) "Cluster-Step and Cluster-Cluster Coalescence... in Ag/Ag(100)", 44th AVS, San Jose, CA, October, 1997.

(T) "Temperature Dependence of Metal(100) Homoepitaxial Growth", APS, Kansas City, Mar 1997.

(S) "Chemical Waves in Surface Reactions", Physical Chemistry Seminar, ISU, October, 1996.

(T) "Submonolayer..Growth & Multilayer Kinetic Roughening...for Ag/Ag(100)", 10th ACCG, Vail, CO Aug 1996.

(P) "Non-Linear Diffusion and Wave Propagation in Surface Reactions", SIAM, Kansas City, July, 1996.

(P) "Spatiotemporal Behavior in Surface Reactions", 10th DOE Confe Catalysis/Surface Chem, Texas, May, 1996.

(T) "Spatiotemporal Behavior in Catalytic Surface Reactions", Ames Lab Chem. Sci. Review, May, 1996.

(T) "Microscopic Models for Chemical Waves in Surface Reactions", 42<sup>nd</sup> AVS, Minneapolis, Oct 1995

(T) "Interface Propagation and Nucleation Phenomena for First-Order Poisoning Transitions," Symp. on "Phase Transitions in Catalytic Surface Reaction Models," IMA, U. Minnesota, June 1994. (1 hr talk).

(P) "Spatiotemporal Behavior in Surface Reactions," 9th DOE Conf. Catalysis/Surface Chem, WI, May 1994.

(S) "Modeling of Spatiotemporal Behavior in Surface Reactions," Ames Lab Chem Sci Prog Review, May 1993.

(T) "Irreversible Island Formation during Deposition: Sizes, Separations, etc," March APS, Seattle, 1993.

(S) "Modeling Surface Reactions: Reaction-Diffusion Equn vs Stochastic Models," Math ISU, Dec. 1992.

(P) "Irreversible Island Formation in Surface Deposition: Sizes & Separations", MRS, Boston, Nov. 1992.

(T) "Island Separation Scaling in Non-Equilibrium Surface Deposition," 39th AVS, Chicago, Nov. 1992.

(P) "Island Size Scaling in Surface Diffusion Processes," STATPHYS-18, Berlin, August, 1992.

(T) "Kinetic Phase Diagrams for Surface Reactions: Unification of MF and LG Behavior," ibid, 1992.

(T) "Relationship between Film Growth Mech., Roughening & Bragg Oscillation Decay," APS, Indiana, Mar. 1992

(T) "Hybrid Model for CO-Oxidation on Surfaces: Mean-Field CO and Lattice-Gas O," ibid, Mar. 1992.

(P) "Spatiotemporal Behavior in Surface Reactions," 8th DOE Conf Catalysis/Surface Chem, CA, March 1992.

(S) "Kinetic Phase Transitions, Catalytic Reactions, Epidemics," Math Physics, ISU, May 1991.

(T) "Epidemic Picture of Kinetics at 1st Order Catalytic Poisoning Transition," APS, Cincinnati, Mar 1991.

(T) "Interface Scaling applied to Models for Low-T Epitaxial Growth on fcc(100) Substrates," ibid, 1991.

(T) "Interface Scaling for Analysis of Low-T Epitaxial Growth," AVS MN Ch., Minneapolis, Feb. 1991.

(T) "Kinetics near 1st Order Poisoning Transition," 5th LASST Workshop Interface Phenom, Bar Harbor, Aug 1990.

(P) "Percolative Structure in Chemisorption & Epitaxial Growth," GRC - Fractals, Plymouth, Aug, 1990.

(P) "Downward Funneling Model of Low-Temp. Epitaxial Growth," 3<sup>rd</sup> Int. ISCC, UW-Milwaukee, July 1990.

(T) "Characterizing the Evolution of Non-Equilibrium Structure During Adsorption," ibid, July 1990.

(S) "Equilibrium vs Non-Equilibrium Structure: Cl/Ag(100) vs O/Fe(100),"Phys. Chem., ISU, Mar 1990.

### CONTRIBUTED CONFERENCE TALKS (T), POSTERS (P), AND ISU SEMINARS (S): (cont.)

(S) "Low-Temperature Epitaxial Thin-Film Growth," Solid State Physics Seminar, ISU, Nov 1989.

(S) "Modeling Adsorption Processes: Structure and Kinetics," Math Dept Colloquium, ISU, Sept 1989.

(T) "Low-Temp. Epitaxial Growth: Influence of Adsorption Site Geometry," APS, St. Louis, Mar 1989.

(S) "Non-Equilibrium Microstructure of Surface Adlayers," Solid State Physics Seminar, ISU, Oct 1988.

(P) "Percolative Aspects of Non-equilibrium Adlayer Structure," 34<sup>th</sup> AVS, Anaheim, Nov. 1987.

(P) "Multi-Cluster Growth on Lattices via Cooperative Filling," STATPHYS-16, Boston U., Aug. 1986.

(T) "Multi-Cluster Growth via Irreversible Cooperative Filling," UC Stat. Mech. Mtg, Davis, Mar. 1986.

(S) "Kinetics & Statistics of Clustering, Growth and Aggregation Processes," Chemistry, ISU, Sept. 1985.

(S) "Irreversible Cooperative Adsorption & Reaction Processes," Solid State Physics, ISU, Mar. 1985.

(T) "Irreversible Random & Cooperative Processes on Lattices," 51<sup>st</sup> Stat. Mech. Mtg Rutgers, May 1984.

(T) "Irreversible Adsorption onto Lattices: Spatial Corr. etc," 16<sup>th</sup> Midwest Theo. Chem. Conf., NWU, May 1983.

(P) "Factorization Relations etc for Dissociative Collisions," 15th Midwest Theo Chem Conf, Mich SU, April 1982.

(P) "Reactive Quantum Boltzmann Eqn from ACQM," GRC - Few Body Problems, Wolfeboro, August 1981.

(P) "Non-Equil. Adlayers from Irreversible Chemisorption," Int. Conf Phase Trans Surfaces, U. Maine, Aug 1981.

(P) "Factorization Relations etc in the Sudden Approx," 14th Midwest Theo Chem Conf., U. Chicago, May 1981.

(P) "Exact Solution for some IVP's in Kinetic Theory," 14th Int. Conf. Thermo & Stat Mech, Edmonton, Aug 1980.

(T) "Exact Results for Non-Equilibrium Models of Surface Adsorption," ibid, Alberta, August 1980.

(T) "Reactive Quantum Boltzmann Equation from Arrangement Channel BBGKY Hierarchy," ibid, 1980.

(S) "The Kinetics of Chemically Reactive Systems," Physical Chemistry Seminar, ISU, March 1980.

(P) "Completeness for Faddeev Equations in Differential Form," GRC-Few Body Problems, Wolfeboro, Aug 1979.

### SERVICE AND PROFESSIONAL ACTIVITIES:

### **<u>REFEREE FOR THE FOLLOWING JOURNALS</u>:**

Science J. Mathematical Physics J. Statistical Physics J. Physical Chemistry Langmuir Theoretical Chimica Acta Applied Physics A J. Vacuum Science & Tech. J. Applied Physics New J. Physics Philosophical Magazine Discrete Contin. Dyn. Sys. B Physical Review Letters J. Chemical Physics Physical Review E Physical Review B Surface Science Physics Letters A Europhysics Letters Chemical Physics Letters Thin Solid Films MRS Proceedings Canada J. Physics

Chaos J. Crystal Growth Physica D Chemical Physics J. Colloids and Surfaces A Vacuum J. Catalysis Physica A Euro. J. Physics B J. Low Temp. Physics J. Zhejiang U. Sci. A

### **REVIEWER FOR THE FOLLOWING FUNDING AGENCIES**:

National Science Foundation (USA) U. S. Department of Energy (BES) Petroleum Research Foundation (ACS). International Science Foundation (USA) Research Corporation Austrian Science Foundation Israel Science Foundation Maine Science & Technology Foundation

### LEVEL OF RECENT REVIEWING ACTIVITY:

- 1992: reviewed 17 journal papers (including 2 revisions)
- 1993: reviewed 15 journal papers (including 3 revisions), 1 proposal.
- 1994: reviewed 19 journal papers (including 4 revisions), 2 proposals, 1 tenure case.
- 1995: reviewed 18 journal papers (including 3 revisions), 2 NSF proposals.
- 1996: reviewed 19 journal/proceedings papers (incl. 3 revisions), 4 proposals, 1 promotion case.
- 1997: reviewed 23 journal papers (including 4 revisions), 5 proposals, 2 award nominations.
- 1998: reviewed 21 journal papers (including. 5 revisions), 1 proposal.
- 1999: reviewed 23 journal papers (including 4 revisions), 2 proposals, 1 tenure case.
- 2000: reviewed 15 journal papers (including 1 revision), 1 NSF proposal.
- 2001: reviewed 23 journal papers (including 2 revisions), 2 NSF proposals, 1 DOE proposal, 1 award nomination.
- 2002: reviewed 20 journal papers (including 2 revisions), 3 NSF proposals, 1 DOE proposal, 1 Research Corp. proposal, 2 tenure or promotion cases
- 2003: reviewed 27 journal papers, 1 NSF proposal, 1 DOE proposal, 1 promotion case.
- 2004: reviewed 19 journal papers
- 2005: reviewed 20 journal papers, 2 NSF, 1 DOE proposal, 9 DOE H-initiative proposals
- 2006: reviewed 18 journal papers, 1 book proposal, 1 NSF proposal
- 2007: reviewed 17 journal papers, 2 NSF proposals, 2 DOE Incite proposals
- 2008: reviewed 10 journal papers (to 6/08), 1 NSF Career Award.

### **SERVICE: ISU MATHEMATICS DEPARTMENT**

### **CURRENT:**

Member of the Tenured Faculty Review Committee: 2008-2009 Member of the IRT for promotion of D. D'Alessandro: 2008-2009 **PREVIOUS:** Member of the IRT for promotion of S. Sethuraman: 2007-2008 Member of the Tenured Faculty Review Committee: 2007-2008 Chair of the IRT for promotion of H. Liu: 2006-2007 Self-study Coordinator for Numerics, Control, and Modeling Research Group 2006-2007 Member Computational Applied Mathematics Search Committee: 2005-2006 Member of the Tenured Faculty Review Committee: 2005-2006 Member Mathematics Dept. DEO Advisory Committee: 2004-2005 Member of the IRT for tenure of H. Liu: 2004-2005 Member of the Tenured Faculty Review Committee: 2004-2005 Member Mathematics Dept. DEO Advisory Committee: 2003-2004 Member Computational and Applied Mathematics Search Committee - cancelled: 2003-2004 Member Applied Mathematics Search Committee: 2002-2003 Chair of the Individual Review Team (IRT) for Untenured Professors: 2001-2002. Chair of the Hiring Committee for the Probability and Stochastic Processes Search: 2001-2002. Chair of the IRT for Untenured Professors: 2000-2001. Member of the IRT for tenure and promotion of X. Wang: 2000-2001. Member of the Individual Review Team (IRT) for Assistant Professors: 1999-2000. Member of the IRT for promotion of S. Hou: 1999-2000. Chair of the IRT for Associate Professors: 1998-99. Member of the Search Committee for an Applied Mathematics Faculty Hire: 1998-99. Member of IRT for promotion of Q. Du: 1998-99. Mentor for Assistant Professor Timo Seppalainen: 1996-98. Member of the IRT for Associate Professors: 1997-98; 1996-97. Chair of Computer Committee: 1997-98; 1996-97. Member of Graduate Committee: 1995-96; 1994-95; 1993-94. Member of Graduate Student Admissions Committee: 1995-96; 1994-95 Member of Faculty Improvement Leave (FIL) Awards Committee: 1993-94.

### SERVICE: PROGRAM OF STUDY (GRADUATE DEGREE) COMMITTEES

### Chair of POS Committee (current):

Xiaofang Guo (Ph.D. Physics/Appl Math 2004-) David Ackerman (Ph.D. Chem. 2008-)

### **POS Committee Member (current):**

Cihan Erbas (Ph.D. EECPE 2006- + Applied Math Minor)					
Xiaolang Xie (Ph. D. Math 2006-)	Luke Roskop (Ph.D. Chem 2006-)				
K.C. Lau (Ph.D., Chem.; 2000-)	Erning Zhang (Ph.D., Chem.; 2000-)				
Toni Smith (Ph.D. Chem 2005-)	Pooja Arora (Ph.D., Chem, 2005-)				
Jerrod Hausser (Ph.D. ChemE, 2005-)	Jun Li (Ph.D Physics 2006-)				
Andrew Severen (Ph.D. MolBio 2005-)	Feng Wei (Ph.D. Physics Lajoie)				
Mingmin Shen (Ph.D. Chem 2005-)	Yingzhou Du (Ph.D. Physics McQueeney)				
Jizhou Chen (Ph.D. Physics Tringides)	Sean Ned (Ph.D. Chem Gordon)				
Jian Zhang (Ph.D. Physics Ho)	Xiao Ma (Ph.D. ME)				
Chad Yuen (Ph.D. Chem. Thiel)	Zachary Royer (Ph.D. Eng.)				

#### Chair of POS Committee (previous):

T. R. Ray (Ph.D., Math; 1991-1994), C. J. Westermeyer (M.Sc., Math; 1994-1995), K.J. Caspersen (Ph.D, Chem; 1999-2001),

#### **POS Committee Member (previous):**

J. M. Fastenau (M.Sc., EE; 1992-93), R. Formas (M.Sc., Physics; 1992-93), J. Jensen (Ph.D., Chem.; 1992-96), B. Diesslin (Ph.D., Math.; 1993-94), D. Koutoudis (Ph.D., Physics; 1993-98), T. L. Pe (Ph.D., Physics; 1994-97), J. McDonald (Ph.D., Physics, 1995-97), K. Stanley (Ph.D., Physics; 1996-97), M. Ifti (M.Sc., Physics, 1997). K.R. Glaesemann (Ph.D., Chem.; 1995-98), D. Federov (Ph.D., Chem; 1996-1999), B. Olson (M.Sc., Math, 1998- Incomplete.) Conrad Stoldt (Ph. D., Chem.; 1997-99), Y. Zhang (Ph.D, Physics; 1995-), X. Jiang (Ph.D., Physics, 1999-2001), C. Song (Ph. D., Physics; 1998-2001), T. Layson (Ph.D., Chem.; 1998-2001), J. Poock (M.Sc., Chem.; 1999-2001), M. Matsuzuki (M.Sc. Chem, 2002), F.-C. Chuang (Ph.D., Physics, 2000-2003) N. Sinha (M.Sc., ChemE, 1998-?), Eun-Yon Kim (M.Sc, Math, 2002-) M. Matsuzuki (Ph.D. Chem, 2002-4) E. Simsek (Ph.D., MS&E, 1998-?), Christine Aitkens (Ph.D., Chem, 2001-2005) Sergev Varangov (Ph.D., Chem, 2001-7) Bosilijka Njegic (Ph.D. Chem. 2005-8) Nick Suek (Ph.D. ChemE, 2005-8)

M. Tammaro (Ph.D., Physics; 1993-1997), E.W. James (Ph. D., Math; 1998-1999).

M. Albao (Ph.D., Physics; 2001-)

B. Kelly (M.Sc., Physics; 1992-93), T. Windus (Ph.D., Chem.; 1992-93), Nguyen Kiet (Ph.D., Chem.; 1992-94), A. Abd El-Hady (Ph. D., Physics; 1993-98), J. Partee (Ph.D., Physics; 1993-97), F. Wilmore (M.Sc., Chem E.; 1995), M. Toutounji (Ph.D., Chem.; 1995-98), F. N. Sheikh (M. Sc., ChemE; 1996), R. Campero (Ph.D., ChemE: 1996-98). N. Kumar (Ph. D., ChemE; 1996-98), A. Hoover (M.Sc., Math.; 1998-99). T.G. Konshak (Ph.D., Chem.; 1995-2005), V. Glezakou (Ph.D., Chem.; 1999-2000), X. Wang (Ph.D., Physics; 1995-), Y. Jung (M.Sc. Chem, 2001) X. Zhu (Ph.D., ChemE, 1998-2001), M. Freitag (Ph.D., Chem.; 1998-2002), M. Pak (Ph. D., Chem; 1997-2002), R. Huang (Ph. D., ChemE; 1998-2003), V. Yeh (Ph.D, Physics, 2000-2003) I. Adamovic (Ph.D. Chem., 2000-4) Ioannis Rousochatzakis (Ph.D. Physics 2003-) Sangwook Wu (Ph.D., Physics, 2001-2005) J. Rintelman (Ph.D., Chem.; 1999-2004), J. Bentz (Ph.D., Chem, 2002-2005) M. Pai (Ph. D. ME 2006-7) (+Appl Math) Deb Zorn (Ph.D. Chem 2005-8)

### Final Oral Committee Member (previous):

G.-L. Zhao (Ph.D., Physics; 1993), C. Kelchner (Ph. D., Chem; 1996). D. Beal (M.Sc., Physics; 1993), T.-Z. Chan (Ph.D. Physics; 2005).

#### **SERVICE: AMES LABORATORY - USDOE**

Chair of Promotion Committee for Brett Bode from Assoc. Scientist (P17) to Scientist I (P18): 2006-7 Chair of Promotion Committee for Slava Dobrovitski from Assoc. Sci. (P17) to Scientist I (P18): 2004-5. Chair of Promotion Committee for Vladimir Kogan from Scientist (P18) to Senior Scientist (P19): 2001. Chair of Promotion Committee for Ozer Unal from Assoc. Scientist (P17) to Scientist I (P18): 1999-2000.

### SERVICE: GENERAL UNIVERSITY

Member of Steering Committee for starting Graduate Certificate in Applied Scientific Computing 2008. Member of Search Committee for Physics Faculty Hire in Condensed Matter Theory 2001-2002. Member of Provost's Committee to Review Proposals for Study in a Second Discipline: 2001-2002 Member of Provost's Committee to Review Proposals for Study in a Second Discipline: 2000-2001 Member of review panel for Pioneer-Hybrid Grants supporting ISU Comp. Mol. Bio.: 1999-2000. Member of review panel for Pioneer-Hybrid Grants supporting ISU Comp. Mol. Bio.: 1998-1999. Faculty Advisor, ISU Badminton Club, 1980-present.

Faculty Advisor, ISU Latin America Solidarity Committee, 1987-94.

Setup/monitor Faculty-Staff payroll deduction for ISU Black South African Student Scholarship Fund.

### **SERVICE: SCIENTIFIC COMMUNITY**:

Co-organizer: SIAM 2008 Materials Science Conference Mini-symposium on "Clustering, Coagulation, and Coarsening Dynamics". Co-organizers: Bob Pego, Barbara Niethammer

Participant of DOE Workshop on "Computational Needs in Alternative & Renewable Energy (CRNARE)", Rockville MD September 2007.

Member of Review Panel for USDOE Basic Research in Hydrogen Fuel Initiatives in the sub-area "Design of Catalysts at the Nanoscale", Rockville, MD, March 2005.

Lead Organizer for the Fall 2004 Materials Research Society Meeting Symposium JJ on "Modeling of Morphological Evolution at Surfaces and Interfaces". This 3.5 day symposium with 91 presentations was dedicated to the memory of Maria C. Bartelt (Scientific Leader for Computational Materials Sciences, CMS Division, Lawrence Livermore NL, and a former postdoc). Co-organizers: Z. Zhang, M. Asta, C. Orme

Co-editor of MRS e-Proceedings Vol. 859E for F2004 MRS Symposium JJ. http://www.mrs.org/publications/epubs/proceedings/fall2004/jj/index.html

Senior (external) examiner for the Ph.D defense of Dogan Uner at Chalmers University, Goteburg, Sweden, March 2003. Topic: Initial Oxidation Kinetics of Al(111): A Monte Carlo Study.

Co-Organizer of American Physical Society (Division of Materials Physics) 2003 March Meeting Focus Session on "Morphological Evolution of Nanostructures, Interfaces, Surfaces, and Thin Films" with R. Phaneuf, R.Q. Hwang, and T.L. Einstein.

Co-Organizer of Materials Research Society Fall 2001 Symposium T on "Statistical Mechanical Modeling in Materials Science" with M.C. Bartelt, A. Karma, S. Torquato, and D. Wolf.

Co-editor of MRS e-Proceedings Vol. 701 for F2001 MRS Symposium T. http://www.mrs.org/publications/epubs/proceedings/fall2001/t/

Co-Organizer of Materials Research Society Spring 2000 Symposium L on "Recent Developments in Oxide and Metals Epitaxy" with M. Yeadon, S. Chiang, R.F.C. Farrow, and O. Auciello.

Co-editor of MRS Proceedings Vol. 619 for S2000 MRS Symposium L.