

## RESUME

### DEPARTMENT OF PHYSICS AND ASTRONOMY IOWA STATE UNIVERSITY

(September 2024)

**NAME: JAMES WILLIAM EVANS**

**TITLE: PROFESSOR**

**B BASE  
GRAD. FACULTY - FULL**

Address: Department of Physics & Astronomy (505 Zaffarano Hall, 2334 Pammel Drive),  
Iowa State University, Ames Iowa 50011  
Telephone: (515)294-1638 Fax: (515)294-4709 Email: evans@ameslab.gov  
Web page: <http://www.ameslab.gov/users/jevans>

#### PERSONAL HISTORY (EDUCATION)

B.Sc. (1<sup>st</sup> Class Honors) - Mathematics (Physics minor) University of Melbourne, Australia 1975  
Ph.D. - Mathematical Physics (advisor: H.S. Green) University of Adelaide, Australia 1979  
Postdoctoral Fellow - Chemical Physics (advisor: D.K. Hoffman) Iowa State U/Ames Lab. 1979-1982

#### PERSONAL HISTORY (PROFESSIONAL EXPERIENCE)

2010-present Professor, Department of Physics & Astronomy, Iowa State University  
1991-present Professor (1996-present), Associate Professor (1991-1996),  
Department of Mathematics, Iowa State University  
2008-present Professor of Physical Chemistry (Graduate Faculty), Iowa State University  
1982-present Project Leader (2004-present); (Sr.) Faculty Scientist (1996-present); Chemist (1993-96),  
Assoc. Physicist (1983-93), Assistant Chemist II (1982-83),  
Division of Chemical & Biological Sciences, Ames Laboratory – USDOE  
2009 Visiting scientist IMA-UMN Minneapolis (March-May), IOP-CAS Beijing (June).  
2000 Visiting Prof., Ecole des Mines/Univ. Henri Poincare Nancy I, France (Summer)  
1991 Visiting Scientist, Fritz Haber Institut der MPG, Berlin, Germany (Summer)  
1989-1991 Adjunct Associate Prof., Departments of Mathematics and Physics, Iowa State University

#### MEMBERSHIPS, HONORS, EDITORIAL BOARDS

Member, American Physical Society (APS)  
Member, Society for Industrial and Applied Mathematics (SIAM)  
Member, American Vacuum Society (AVS): Science & Technology of Materials, Interfaces, Processing  
Member, Editorial Board, Journal of Chemical Physics (American Institute of Physics) (2013 - 2015)  
Member, Editorial Board, Computational Materials Science (Elsevier) (2014-2017)  
Member, Editorial Board, Surface Science (Elsevier) (2015-present)  
Member, Editorial Board, Nanomaterials (MDPI) (2020-present)  
Fellow, American Physical Society – Division of Condensed Matter Physics (2002-present)  
American Physical Society (APS) Outstanding Referee 2015

## PERFORMANCE IN TEACHING POSITION RESPONSIBILITIES

### STATEMENT OF TEACHING PHILOSOPHY

My courses have primarily involved teaching mathematical methods, and theory and modeling strategies for physical systems to audiences of students from a diverse range of disciplines. Specifically, most students have come from physics, chemistry, and various engineering disciplines. My guiding philosophy has been to present the material in a way targeted to the audience (e.g., avoiding unnecessarily abstract and rigorous derivations or proofs in math courses), and wherever possible selecting examples and applications from the students' fields of interest. However, I do aim to provide the students with a complete and solid understanding of the mathematical and theoretical concepts and results, including a self-contained set of lecture notes and supplementary material available on the web. This solid understanding is important in an era where computational modeling is common in applied disciplines, particularly with the aid of "black box" software, but where students' understanding of the underlying theory and mathematical formulations is often incomplete. Input from and interaction with the students during class is encouraged as this invariably provides insight into the student's level of understanding of the material. Such interaction not only enhances learning, but also guides discussion towards topics or issues of particular interest to the students.

Evaluation of students in these courses is based primarily on their performance in closed-book exams (2 or 3 exams during the semester, as well as a comprehensive final). The relative weight of these exams etc., towards the final grade is announced at the beginning of the semester. The exams include questions based primarily on lecture materials and associated homework, so that typical students if diligent should be able to perform reasonably. A sufficient number of questions are included so that failure to answer one question will not severely impact the overall grade on the exam. To challenge stronger students, usually at least one more difficult question is included in each exam.

### LIST COURSES TAUGHT IN LAST ~TEN YEARS, USING A TABULAR FORMAT.

Assignments Sem & Yr	Course	Title	Approx. No. Students
Spring 2024	Phys 564	Advanced Classical Mechanics	12
Fall 2023	Phys 528	Math Methods Phys Sciences	7
Spring 2023	Phys 564	Advanced Classical Mechanics	12
Fall 2022	Phys 528	Math Methods Phys Sciences	13
Spring 2022	Math/Phys 646	Math Model Complex Phys Sys	5
Fall 2021	Phys 528	Math Methods Phys Sciences	23
Fall 2020	Phys 528	Math Methods Phys Sciences	13
Spring 2020	Math/Phys 646	Math Model Complex Phys Sys	5
Fall 2019	Phys 528	Math Methods Phys Sciences	18
Spring 2019	Math/Phys 646	Math Model Complex Phys Sys	7
Fall 2018	Phys 528	Math Methods Phys Sciences	14
Spring 2018	Math/Phys 646	Math Model Complex Phys Sys	14
Fall 2017	Phys 528	Math Methods Phys Sciences	11
Spring 2017	Math/Phys 646	Math Model Complex Phys Sys	7
Fall 2016	Phys 528	Math Methods Phys Sciences	24
Spring 2016	Phys 646	Math Modeling of Complex Phys Sys	7
Spring 2016	Phys 490	Independent study: Stochastic Spatial Processes	1
Fall 2015	Phys 528	Math Methods Phys Sciences	25
Spring 2015	Phys/Math 646	Math Model Complex Phys Sys	5
Fall 2014	Phys 528X	Math Methods Phys Sciences	22
Spring 2014	Phys 646	Math Model Complex Phys Sys	11

<b>Spring 2014</b>	Phys 242 (1/H1) Rec	Classical Phys II (H/LC)	19
<b>Spring 2014</b>	Phys 242 (2/H2) Rec	Classical Phys II (H/LC)	14
<b>Fall 2013</b>	Phys 528X	Math Methods Phys Sciences	18
<b>Spring 2013</b>	Phys 646	Modeling of Cx Physical Systems	12
<b>Fall 2012</b>	Phys 528X	Advanced Math Methods for Physics	23
<b>Spring 2012</b>	Phys 646	Modeling of Cx Physical Systems	18
<b>Fall 2011</b>	Phys 426	Mathematical Methods for the Physical Sciences	25
<b>Spring 2011</b>	Math 646	Math Modeling of...Complex Systems	6
<b>Fall 2010</b>	Math 426	Math Methods for Physical Sciences	21
<b>Spring 2010</b>	Math 646	Math Modeling of...Complex Systems	19
<b>Fall 2009</b>	Math 426	Math Methods for Physical Sciences	28

**SUMMARIZE RESULTS OF STUDENT EVALUATIONS FOR ALL COURSES IN THE LAST ~TEN YEARS ON THE TWO STANDARD QUESTIONS.**

sem/Yr	Course	Sect	Type	Students		Instructor		Course	
				Total Enrolled	% Responded	Overall Rating	Dept Mean for like Instructors	Overall Rating	Dept Mean for like Courses
S24	564		Lec	12	75	4.88		4.56	
F23	528		Lec	7	86	4.83		4.83	
S23	564		Lec	12	75	4.67		4.33	
F22	528		Lec	13	69	4.56	4.5	4.67	4.4
S22	646		Lec	5			4.6		4.5
F21	528		Lec	23	70	4.6	4.5	4.3	4.4
F20*	528	1	Lec	13	92			3.83	
S20*	646	1	Lec	5	66	4.7	4.6	4.3	4.5
F19	528	1	Lec	18	44	4.4	4.6	4.1	4.5
S19	646		Lec	7	57	5.0	4.4	4.5	4.3
F18	528		Lec	14	62	5.0	4.5	4.75	4.3
S18	646		Lec	14	50	4.57	4.5	4.0	4.3
F17	528		Lec	15	73	4.36	4.5	4.18	4.3
S17	646		Lec	7	71	4.8	4.5	4.6	4.3
F16	528		Lec	24	63	4.7	4.5	4.5	4.3
S16	646		Lec	7	100	4.6	4.6	4.3	4.4
F15	528		Lec	25	76	4.7	4.4	4.5	4.4
S15	646		Lec	5	80	4.8	4.6	4.3	4.4
F14	528		Lec	22	82	4.9	4.4	4.8	4.4
S14	646		Lec	11	73	5.0	4.1	4.8	4
S14	242	1/H1	Rec	19	58	3.8	3.9	2.9	3.3
S14	242	2/H2	Rec	14	57	4.0	3.9	3.9	3.3
F13	528X		Lec	18	72	4.3	4.2	4	4.2

sem/Yr	Course	Sect	Type	Students		Instructor		Course	
				Total Enrolled	% Responded	Overall Rating	Dept Mean for like Instructors	Overall Rating	Dept Mean for like Courses
S13	646		Lec	12	67	4.9	4.2	4.6	3.9
F12	528		Lec	23	83	4.5	4.3	4.1	4.1
S12	646		Lec	18	78	4.7	4.3	4.6	4.1
F11	426		Lec	26	85	4.5	4.1	4.2	3.9
S11	646		Lec	6	67	4.5		4.3	
F10	426		Lec	21	71	4.5		4.3	
S10	646		Lec	19	89	4.6		4.5	
F09	426		Lec	28	89	4.6		4.1	

\*Evaluations affected by Covid-19 pandemic

## COURSE AND CURRICULUM DEVELOPMENT ACTIVITY

Phys/Math 646: Mathematical Modeling of Complex Physical Systems (formerly Math 527). I developed this graduate course 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; coarse-grained/macroscale models. This course was designed to meet the interests and key research needs of graduate students in the mathematical, physical, and chemical sciences, and increasingly in various engineering disciplines. It focuses on mathematical theory/formalism underlying the modeling strategies – rather than on code implementation (the focus of other courses) – given that the former is key to reliable analysis. Course material is necessarily drawn from numerous sources, but the presentation is a self-contained, and is accessible to students with various backgrounds (a significant challenge as students come from up to 8 programs in a given year). There has been sufficient interest to run the course every year that it has been offered, most of whom have come from departments other than my own. I believe that this reflects well on the value of the course to a broad clientele (as appreciated by students & faculty).

Phys 528: (Advanced) Mathematical Methods for the Physical Sciences. This course was developed and offered for the first time in Fall 2012 after extensive discussions with the Physics Curriculum Committee in Spring 2012. The philosophy was to significantly “enhance” the lower level course Math/Phys 426 to cover key additional topics of relevance to the Graduate Physics Core Curriculum (Hilbert spaces, linear operators, more emphasis on ODE’s and PDE’s central to physics, etc.), as well as to increase the level of difficulty of the material. Thus, the content and level of presentation in 528 differs greatly from 426.

Phys 564: Advanced Classical Mechanics. Upon first teaching this course in Spring 2023, I refined the standard course syllabus which followed the classic text by Goldstein. Connection of basic concepts in the text was made to modern Molecular Dynamics (MD) simulations (which utilize a significant portion of national supercomputing resources). Many-body vs just pair-wise potentials were discussed (a serious deficiency of Goldstein). Stochastic Langevin dynamics (not covered by Goldstein) was also reviewed.

## HONORS AND AWARDS RECEIVED FOR TEACHING

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

Most Graduate Valuable Instructor Award for 2022: ISU Physics Grad Student Assoc. Award

**UNDERGRADUATE ADVISING.**

a. Average number of advisees per year since ~2014 \_\_6\_\_.

**NSF REU Undergraduate Trainees:**

Kasey Mathess 2002; Bethany Weinert 2003; Daniel Unruh 2004 (went to grad school then postdoc); Kyle Schnitzenbaumer 2005-6 (went to graduate school), Kyle Mandsager 2007 (went to medical school).

**Ames Laboratory USDOE Undergraduate Research Trainees - SULI program:**

John A. Bartz 1986; J.A. Rabaey 1988; Mark S. Miesch 1990 (now an NCAR Scientist); Mel Sabella 1992; Joey Wendel 2010; Tyler Pleasant 2018 (now in grad school); Xin (Jason) Zhang 2021 (JHU).

**GRADUATE ADVISING****A. PH.D. PROGRAM OF STUDY COMMITTEES (SINCE APPOINTMENT in 1991)****1. In progress (# = number of publications)**

- **Chair/major professor**
- **Member of committee**

Suvadip Mandal (PhysA), Shreeram Jawadekar (Phys Vary) and many others from multiple departments (including Chemistry, Mathematics, multiple Engineering departments)

**2. Completed (# = number of coauthored publications):**

- **Chair/major professor (name, degree, date, # publications, current employer)**

Timothy R. Ray (Ph.D., Applied Math; 1991-1994 # = 2)

– currently NSA analyst; previously Professor, SE Missouri State U.

Michael Tamaro (Ph.D., Physics-CMP; 1993-1997 # = 8)

– Teaching Professor, Physics, U. Rhode Island

Edna W. James (Ph. D., Applied Math; 1998-1999 # = 4)

– Asst. Professor, Mathematics, Algoma U., Canada

Kyle J. Caspersen (Ph.D, Chem; 1999-2001 # = 11)

– Research Scientist, Lawrence Livermore NL

Marvin Albao (Ph.D., Physics-CMP; 2001-2006 # = 8)

– Professor, Physics, U. Philippines Los Banos

Xiaofang Guo (Ph.D. Physics-CMP/Applied Math 2004-2008 # = 7)

– Analyst, I-Behavior

David Ackerman (Ph.D. Chem. 2008-2013 # = 11)

- Research Scientist ISU Computational Mechanical Engineering

Chi-Jen Wang (Ph.D. Applied Math 2009-2013 # = 7)

–Assoc. Prof., Math National Chung Chen University, Taiwan; postdoc GA Tech

Jing Wang (Applied Math 2010-2013 # = 7)

– Senior Data Analyst @ Cambium Assessment (previous Amer Inst. Research)

Andres Garcia (Ph.D. Physics - CMP 2013 – 2017, # = 7)

– Software Engineer, Gamma 1 Technologies (previously lecturer at Drake)

King (Alex) Lai (PhD PhysA 2015-2020, # = 12)

- Humboldt Junior Fellow postdoc at Fritz Haber Inst. – MPG, Berlin

Zheren (Steve) Shen (Ph.D. Applied Math 2019-2023 # = 2)

- Postdoc, mathematics, Shanghai International Studies University

• **Member of committee**

T. Windus (Chem. 1992-93); T. L. Pe (Phys. 1994-97); J. Jensen (Chem. 1992-96)  
 N. Kiet (Chem. 1992-94); B. Diesslin (Math. 1993-94); A. Abd El-Hady (Phys. 1993-98)  
 G.-L. Zhao (Phys. 1993); C. Kelchner (Chem. 1996); D. Koutoudis (Phys. 1993-98);  
 J. Partee (Phys. 1993-97); J. McDonald (Phys. 1995-97); M. Toutounji (Chem. 1995-98)  
 K. Stanley (Phys. 1996-97); R. Campero (ChemE; 96-98); K. Glaesemann (Chem.95-98);  
 N. Kumar (ChemE. 1996-98); D. Federov (Chem. 1996-99); T.G. Konshak (Chem. 95-05)  
 C. Stoldt (Chem. 1997-99); V. Glezakou (Chem.; 1999-2000); Y. Zhang (Phys. 1995-)  
 X. Wang (Phys. 1995-); X. Jiang (Phys. 1999-2001); C. Song (Phys. 1998-2001)  
 X. Zhu (ChemE, 1998-2001); T. Layson (Chem. 1998-2001); M. Freitag (Chem. 98-2002)  
 M. Pak (Chem. 1997-2002); R. Huang (ChemE. 1998-2003); F.-C. Chuang (Phys. 00-03)  
 V. Yeh (Phys. 2000-2003); I. Adamovic (Chem. 2000-04); I. Rousochatzakis (Phys. 2003-)  
 M. Matsuzuki (Chem. 2002-04); S. Wu (Phys. 2001-05); C. Aitkens (Chem. 2001-05);  
 J. Bentz (Chem. 2002-05) ; S. Varangov (Chem, 2001-07); M. Pai (ME 2006-07 +AMath);  
 B. Njegic (Chem. 2005-08); D. Zorn (Chem. 2005-08); N. Suek (ChemE, 2005-08);  
 X. Xie (Math 2006-08); K.C. Lau (Chem.; 2000-); Erning Zhang (Chem. 2000-);  
 Cihan Erbas (EECP/AMath 06-09); M. Shen (Chem 2005-); P. Arora (Chem. 2005-);  
 J. Rintelman (Chem. 1999-2004); T.-Z. Chan (Phys. 2005) ; Jun Li (Phys. 2010-);  
 A. Smith (Chem. 20xx-); Hui Xie (NDE-EE 20xx-); Luke Roskop (Chem. MSG 20xx-);  
 J. Hausser (ChemE 20xx-); Z. Royer (MSE 2012-); Alex Belankinov (Chem 2012-);  
 Sean Nedd (Chem. Gordon 2012-); C. Yuen (Chem. Thiel 13-); Hui Yu (AMath Liu 2013)  
 K. Lord (MSE King 2013); S. Russell (Chem Thiel 2013); D. Appy (Chem Thiel -2014);  
 K. Knorowski (Phys. AT -2015); R. Grandin (ME-NDE -14); B. Estervig (Math Sacks -15);  
 R. Gustav (Phys. Goldman -2014); J. Liao (Phys HEP -2014); S. Liu (AMath MT -2011);  
 D. Shao (Chem. Thiel -2014); J. Zhang (Phys -2010); F. Wei (Phys. NPhys -2010);  
 Dapeng Jing (Chem Thiel -10); G-A Negoita (Phys Vary -10); S. Alvarado (Chem Vela -15)  
 Xin Zhao (Phys -2015); Wenjia Liu (Phys. Schmittman -14); Jizhou Chen (Phys Tringides)  
 Jian Zhang (Phys Ho); Xiao Ma (Ph.D. ME); Zhao Xia (Phys A KM Ho)  
 H. Zhang (Ph.D. Physics Qui); E. Smith (PhD ME Subramanian 17)  
 D. Quirinale (Phys Goldman 17); T.H. Chou (Phys Yu 17); J. Delmar (Phys. Yu/Evans 17);  
 S. Shaw (MSE Cademarti 17); H. Walen (Chem. Thiel 16); E. Kwolek (Chem. Thiel 16);  
 Eric Murphy (ME Baskar G 17); Lee Trask (ChemE Cochran xx); J. Cui (Phys Furakawa);  
 Brian Voas (PhD MSE Beckman 15); Zach Voller (AMath 17); Steve Noren (AMath 18);  
 Spencer Pfeifer (ME Baskar G 17); Balaji Pokuri (ME Baskar G 18) Joani Mato (Chem  
 Gordon); Miles White (Chem. Vela); Kai-Chung Lau (Chem); Peter Spurgeon (Chem  
 Thiel 20 ); Yingzhou Du (Phys McQueeney); Chen Liu (PhD KM Ho); Willam Everett  
 (Chem Windus); Taylor Harville (Chem Gordon); Yi-Ann Lii-Rosales (Chem Thiel 19);  
 Zhuoran Wang (Chem); Viet Nguyen (Song Chem); David Poole (Chem Gordon); Xun Zha  
 (Phys Travesset); Jorge Galvez (Chem Gordon); Raman Noruzi (ME Baskar Ganapathy...);  
 Nate Andersen (Phys Vaknin/Evans); Minda Chen (Chem); Trevor Lyons (MSE  
 Napolitano); Manas Bhatnager (Math H Liu) *and many others currently.*

**B. M.S./M.A. PROGRAM OF STUDY COMMITTEES (SINCE APPOINTMENT)**

**1. In progress:**

- Chair/major professor (list names of students)
- Member of committee (list names of students)

**Completed:**

- **Chair/major professor**

C. J. Westermeyer (M.Sc., Math; 1994-1995)  
 Renjie Zhao (M.Sc. Phys. 2012-2014)  
 Zheren Shen (Applied Math 2018-2019)

- **Member of committee (list names of students)**

J. M. Fastenau (EE; 1992-93); B. Kelly (Phys. 1992-93); R. Formas (Phys. 1992-93);  
 D. Beal (Phys. 1993); M. Ifti (Phys. 1997); A. Hoover (Math. 1998-99);  
 F. Wilmore (ChemE. 1995); N. Sinha (ChemE 1998-); F. N. Sheikh (ChemE; 1996)  
 J. Poock (Chem. 1999-2001); E. Simsek (MS&E 1998-?); Eun-Yon Kim (Math, 2002-);  
 M. Matsuzuki (Chem. 2002); B. Olson (Math. 1998-); Geoff Root (PhysA 2013);  
 Y. Jung (M.Sc. Chem, 2001); F.-C. Chuang (Phys 05); H. Zhang (Phys -2010);  
 A. Severein (AMath -2009); J. Knutson (AMath -2011);  
 H.Q. Phoon (PhysA HE Valencia 15); A Nashleanas (Chem Windus 15);  
 Jiyoung Lee (Chem Windus 18); Michael Manley (Chem Thiel 20)

**C. SUPERVISION OF POSTDOCTORAL FELLOWS AND STAFF SCIENTISTS**

**Postdocs (name, PhD degree, dates at ISU, # publications at ISU, current employer)**

**Current:****Former:**

Dr. Andres Garcia (PhD ISU Physics - CMP 2017 #=7) Software Engineer Gamma 1  
 Dr. King(Alex) C. Lai (PhD ISU 2020) 2020 #=12 Humboldt Jr Fellow, Fritz Haber Institute - MPG  
 Dr. Jing Wang (Ph.D ISU 2013) 2013-2014 # = 7 Senior Data Analyst, Cambrium Assessment  
 Dr. Chi-Jen Wang (Ph.D. ISU 2013) 2013-2014 # = 7 Assoc. Prof. National Chung Chen U, Taiwan  
 Dr. Yong Han (Ph.D Utah 2006) 2007-2010 # > 40 Staff Scientist, Physics & Astronomy ISU.  
 Dr. Maozhi Li (Ph.D.CAS-Beijing 2001) 2001-2005 # = 13 Assoc. Prof. Physics Renmin U., Beijing  
 Dr. Chandana Ghosh (Ph.D. KSU 2004) 2004-2005 # = 4 Engineer @ Siemens, FL.  
 Dr. Da-Jiang Liu (Ph.D. U Maryland 1998) 1998-2001 # > 80 Staff Scientist, Ames Laboratory/ISU  
 Dr. A. M. Cadilhe (Ph.D. Clarkson 1997) 1997-1999 # = 4 U. do Minho/LANL/U Fed. De Minas Gerias  
 Dr. Maria C. Bartelt (Ph.D. Clarkson 1991) 1991-1996 # = 23 Deceased. Formerly Scientific Capability  
 Leader/Directorate of Computational Materials Sci., CMS Lawrence Livermore NL – USDOE  
 Dr. H. Chuan Kang (Ph.D. Caltech 1990) 1990-91 # =6 Assoc.Prof.Chem/Assoc Dean, Nat U. Singapore

**Staff Scientists (name, PhD degree, dates at ISU, # publications at ISU)**

**Current:**

Dr. Da-Jiang Liu (Ph.D. U Maryland 1998) 2001-present # > 90 Ames Laboratory Scientist II DCBS  
 Dr. Yong Han (Ph.D Utah 2006) 2011-present # ~ 50 ISU Research Scientist II

**DEPARTMENTAL SERVICE**

Assistant Department Chair (PhysA) 2024-2025  
 Member: Astro Teaching Faculty Search committee (PhysA) 2024-2025  
 Chair: Promotion Committee for Songting Luo (Math Department)  
 Class scheduling coordinator (PhysA) 2024-2025  
 Chair: Alumni Relations committee (PhysA) 2024-2025  
Member: Undergraduate advising group (PhysA) 2024-2025  
 Assistant Department Chair (PhysA) 2023-2024  
 Chair: Hiring committee for Teaching Prof. in Physics (PhysA) 2023-2024  
 Class scheduling coordinator (PhysA) 2023-2024  
 Member: Lab Tech hiring committee (PhysA) 2023-2024  
 Chair: Alumni Relations committee (PhysA) 2023-2024  
Member: Undergraduate advising group (PhysA) 2023-2024  
 Class scheduling coordinator (PhysA) 2022-2023  
 Inspector General for qualifier exams (PhysA) 2022-2023  
 Chair: Alumni Relations committee (PhysA) 2022-2023  
 Member: Undergraduate advising group (PhysA) 2023-2023  
Member: Hiring Committee for Barton Chair (Chemistry) 2022-2023  
 Class scheduling coordinator (PhysA) 2021-2022  
 Inspector General for qualifier exams (PhysA) 2021-2022  
 Chair: Alumni Relations committee (PhysA) 2021-2022  
 Member: Undergraduate advising group (PhysA) 2021-2022  
Member: Promotion and Tenure Committee for Jue Yan (Math) 2021-2022  
 Member: Undergraduate advising group (PhysA) 2020-2021  
 Class scheduling coordinator (PhysA) 2020-2021  
Member: Modern qualifier exam (for Aug. 2020)  
 Chair: Committee for Spousal Accommodation Hire (PhysA) 2019-2020  
 Member: Undergraduate advising group (PhysA) 2019-2020  
 Class scheduling coordinator (PhysA) 2019-2020  
 Representative: Faculty Senate (for PhysA) 2019-2020  
Chair: Modern qualifier exam (for Aug. 2019)  
 Member: Promotion and Tenure Committee (PhysA) 2018-2019  
 Member: Undergraduate advising group (PhysA) 2018-2019  
 Class scheduling coordinator (PhysA) 2018-2019  
 Theory Cluster Hire – CMP subcommittee (PhysA) 2018-2019  
Representative: Faculty Senate (for PhysA) 2018-2019  
 Member: Promotion and Tenure Committee (PhysA) 2017-2018  
 Chair: Modern qualifier exam (for Aug. 2018)  
 Member: Undergraduate advising group (PhysA) 2017-2018  
Representative: Faculty Senate (for PhysA) 2017-2018  
 Member: Promotion and Tenure Committee (PhysA) 2016-2017  
 Member: Modern Qualifier committee (PhysA) 2016-2017  
 Member: Curriculum Committee (PhysA) 2016-2017  
 Member: Graduate Committee (PhysA) 2016-2017  
 Member: Undergraduate advising group (PhysA) 2016-2017  
Representative: Faculty Senate (for PhysA) 2016-2017  
 Member: Promotion and Tenure Committee (PhysA) 2015-2016  
 Member: Curriculum Committee (PhysA) 2015-2016  
 Member: Graduate Committee (PhysA) 2015-2016  
 Member: Undergraduate advising group (PhysA) 2015-2016



Member: Classical Qualifier regrading committee (PhysA) 2015-2016  
Representative: Faculty Senate (for PhysA) 2015-2016  
 Chair: Hiring committee for Mesoscale Science (PhysA) 2014-2015  
 Member: Hiring committee for Mesoscale Science (Chemistry) 2014-2015  
 Chair: Focus Area Committee (FAC) for hiring in mesoscale science  
 Member: Graduate Committee (PhysA) 2014-2015  
 Member: Undergraduate advising group (PhysA) 2014-2015  
Representative: Faculty Senate (for PhysA) 2014-2015  
 Member: Promotion and Tenure Committee (PhysA) 2013-2014  
 Member: Graduate Committee (PhysA) 2013-2014  
 Member: Undergraduate advising group (PhysA) 2013-2014  
 Member: Promotion and Tenure Committee for Matzavinos (Math) 2013-2014  
Inspector General- Physics Qualifiers (PhysA) 2013-2014  
 Member: Undergraduate advising group (PhysA) 2012-2013  
 Member: Graduate Committee (PhysA) 2012-2013  
 Member: Promotion and Tenure Committee (PhysA) 2012-2013  
 Member: Promotion and Tenure Committee for Matzavinos (Math) 2012-2013  
Member: Modern Qualifier Committee (PhysA) 2012-2013  
 Member: Graduate Committee (PhysA) 2011-2012  
 Member: 3 year review committee for A Matzavinos (Math) 2010-2011  
 Member: Committee for Combinatorics/Computational Math Search (Math) 2009-2010  
 Member of the Tenured Faculty Review Committee (Math) 2009-2010  
 Member: Graduate Committee (Math) Fall 2008  
 Member: Wolfe Award Committee (Math) Fall 2008  
 Member of the Tenured Faculty Review Committee (Math) 2008-2009  
 Member of the IRT for promotion of D. D'Alessandro (Math) 2008-2009  
 Member of the IRT for promotion of S. Sethuraman (Math) 2007-2008  
 Member of the Tenured Faculty Review Committee (Math) 2007-2008  
 Chair of the IRT for promotion of H. Liu (Math) 2006-2007  
 Self-study Coordinator for Numerics, Control, and Modeling Research Group (Math) 2006-2007  
 Member Computational Applied Mathematics Search Committee (Math) 2005-2006  
 Member of the Tenured Faculty Review Committee (Math) 2005-2006  
 Member Mathematics Dept. DEO Advisory Committee (Math) 2004-2005  
 Member of the IRT for tenure of H. Liu (Math) 2004-2005  
 Member of the Tenured Faculty Review Committee (Math) 2004-2005  
 Member Mathematics Dept. DEO Advisory Committee (Math) 2003-2004  
 Member Computational & Applied Math Search Committee – cancelled (Math) 2003-2004  
 Member Applied Mathematics Search Committee (Math) 2002-2003  
 Member of Search Committee in Condensed Matter Theory (PhysA) 2001-2002.  
 Chair of the Individual Review Team (IRT) for Untenured Professors (Math) 2001-2002.  
 Chair of Hiring Committee for the Probability & Stochastic Processes Search (Math) 2001-2002.  
 Chair of the IRT for Untenured Professors (Math) 2000-2001.  
 Member of the IRT for tenure and promotion of X. Wang (Math) 2000-2001.  
 Member of the Individual Review Team (IRT) for Assistant Professors (Math) 1999-2000.  
 Member of the IRT for promotion of S. Hou (Math) 1999-2000.  
 Chair of the IRT for Associate Professors (Math) 1998-99.  
 Member of the Search Committee for an Applied Mathematics Faculty Hire (Math) 1998-99.  
 Member of IRT for promotion of Q. Du (Math) 1998-99.  
 Mentor for Assistant Professor Timo Seppalainen (Math) 1996-98.  
 Member of the IRT for Associate Professors (Math) 1997-98; 1996-97.  
 Chair of Computer Committee (Math) 1997-98; 1996-97.

Member of Graduate Committee (Math) 1995-96; 1994-95; 1993-94.

Member of Graduate Student Admissions Committee (Math) 1995-96; 1994-95

Member of Faculty Improvement Leave (FIL) Awards Committee (Math) 1993-94.

### **AMES LABORATORY SERVICE**

Member: Search Committee, Ames Lab Scientist II for Catalysis project, 2022.

Member: Search Committee, Division of Chemical & Biosciences Director 2018

Member: Computational Instructure Committee: 2017-2018

Member: Ames Laboratory Strategic Planning Committee: 2017

Member: Promotion committee for Igor Slowing from Assoc. Scientist to Scientist I: 2016-2017

Member: Promotion committee for Rana Biswas from Scientist to Scientist II: 2012-2013

Member: Promotion committee for Slava Dobrovistki from Scientist to Scientist II: 2012-2013

Member: Promotion committee for Vladimir Antropov from Scientist to Scientist II: 2012-2013

Member: Promotion committee for Myron Hupalo from Assoc. Sci to Scientist: 2011-2012

Member: Promotion committee for Mikhail Mendelev from Assoc. Sci to Scientist: 2011-2012

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.

### **COLLEGE SERVICE**

Member: LAS Promotion and Tenure Committee 2016-2017

Chair: LAS Promotion and Tenure Committee 2015-2016

Chair: LAS Promotion and Tenure Committee 2014-2015

Member: LAS Complex Materials Workshop planning committee 2014-2015

Chair: LAS Promotion and Tenure Committee 2013-2014

Member: LAS Promotion and Tenure Committee 2012-2013

Member: LAS Promotion and Tenure Committee 2011-2012

### **UNIVERSITY SERVICE**

Member of Steering Committee for Graduate Minor in Applied Scientific Computing 2008-present.

ISU Faculty Senate 2014-2020

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, 1980-2013.

### **EXTERNAL PROFESSIONAL SERVICE**

See listing of Conference Symposium Organization, Editorial Board membership, etc. below.

**RESEARCH HIGHLIGHTS:** CR = Chem Rev (IF=52.6); RMP = Rev Mod Phys (36.9); NL = Nano Lett (12.1); PRL (8.8); SSR = Surf Sci Rep (17.8); PSS = Prog Surf Sci (9.0); JPCL/C = J Phys Chem Lett/C (8.7/4.5); PRB (3.8); JCP = J Chem Phys; SS = Surf Sci; MMS = SIAM Multiscale; PRM = Phys Rev Mat.

### **SELF-ASSEMBLY & STABILITY OF NANOSTRUCTURES, THIN FILM GROWTH**

#### **DYNAMICS OF 3D METALLIC NANOCLUSTERS: RESHAPING, DIFFUSION, ETC.**

◆ Developed the first realistic atomistic-level treatment of the kinetics of surface-diffusion-controlled reshaping including sintering and pinch-off in metallic fcc nanoclusters, diffusion of 3D NCs [CR19].

#### **PREDICTIVE MODELING OF SELF-ASSEMBLY OF SUPPORTED NANOCLUSTERS (NCs)**

◆ Developed a formulation for nucleation and growth of intercalated islands under the surface or layered materials, and performed detailed DFT analysis of energetics for these systems [PRM17, JPCC18, etc]

◆ First detailed atomistic modeling of directed-assembly of metal NC on periodically ruffled graphene supported on Ru(0001) accounting for modulated potential energy surface [PSS15, JCP13, 15, PRB12].

◆ Developed the only formalism incorporating an ab-initio level treatment of kinetics for periphery diffusion and intermixing to reliably describe self-assembly of single and multicomponent NCs; the formalism applied to: Ni+Al on NiAl(110) [PNAS11, JCP11, PRL12] revealing nanoscale Kirkendall voiding; Ag+Au on Ag(100) [NL14]; Au chains on Ag(100)/NiAl(100) [JCPL15].

◆ Quantum size effects [Materials10]: modeling of bilayer Ag island growth on NiAl(110) treating facile upward transport at low T [PRB10, PRL08], and of 3-layer Ag islands on Al-based quasicrystals [PRL09].

◆ Other: starfish islands on 5-fold quasicrystal surfaces [SS06]; metal atomic wires on Si(100) [PRB05]; self-assembly of fat fractals & dendrites including detailed modeling for Ag/Ag(111) [PRB05, SSR06].

#### **2D NANOCLUSTER DIFFUSION, SINTERING, AND DESTABILIZATION (COARSENING)**

◆ Developed fundamental theory and predictive atomistic modeling for nanoscale coalescence/sintering and cluster diffusion [CR19, JPCC18, PRB17, JPCC16, NL14, PRB02, PRL01, PRL98]: explained role of kink rounding barrier inducing anomalous scaling with size for cluster-cluster and cluster-step sintering phenomena, and developed corrected scaling theories for edge nucleation-limited cluster diffusion.

◆ Developed non-linear reaction-diffusion equation theory for additive(S)-enhanced coarsening on M(111) surfaces; identified  $MS_2$  and  $M_2S_3$  complexes as dominant mass carriers [SS18, PRB15, Science10, JCP09].

◆ Anisotropic coarsening: developed analytic formulation and atomistic models for anomalous coarsening of rectangular islands with non-equilibrium shapes (constant width) in metal(110) systems [2×PRB13]

◆ Analysis of competition between Ostwald Ripening (OR) and Smoluchowski Ripening (SR) pathways [JPCC09] following our identification of SR as the dominant pathway for metal(100) systems [PRL96].

#### **BEYOND-MEAN-FIELD (MF) NUCLEATION THEORY FOR THIN FILM GROWTH [SSR06]**

◆ Developed a precise beyond-mean-field nucleation theory for the classic problem of island formation on surfaces during deposition [JCP16, PRB96, SS93, PRB92] which corrects classic MF Venables theory. Identified subtle correlations between islands size and separation (or capture zone area) as origin of the failure of MF theory, a feature supported by our analysis of experimental data [PRL98, PRB99].

◆ Simulation of optimally tailored models (with point, square,.. islands) for first precise determination of island size distribution (ISD), island spatial correlations, adlayer percolation, transitions in critical size, effects of anisotropic diffusion, small-cluster diffusion [PRB96, SS95, PRL94, SS93, ...].

◆ Rigorous formulation of capture zone (CZ) area distributions based on accurate description of key spatial aspects of nucleation [JCP16,PRL10]. Realistic formulation for the Joint Probability Distribution of island sizes and CZ areas, providing the most complete description of nucleation [PRB02,PRB01].

◆ Developed Geometry-Based Simulation (GBS) algorithm exploiting a “stochastic geometry” picture of island formation for optimally efficient simulation when treating larger critical sizes [MMS05,PRB03]

### **MULTILAYER EPITAXIAL GROWTH: KINETIC ROUGHENING & MOUND FORMATION**

◆ Introduced “downward funneling” explaining smooth growth in metal systems @ low T [SS06,PRB90].

◆ First predictive modeling of kinetic roughening with mound slope selection for Fe/Fe(100) [PRL95]. Most comprehensive predictive modeling of T-dependent mound formation and coarsening for M/M(100) systems [PRB02,PRB01,PRL00], and of fractal wedding-cake formation for Ag/Ag(111) [PRB08].

◆ Coarse-graining of step dynamics revealed limitations of heuristic PDE’s for unstable growth [PRL05].

◆ Refined mesoscale BCF theories: coarse-graining of discrete deposition-diffusion equations produces kinetic coefficients and permeabilities correcting traditional (Chernov) BCs [PRB16,PRB15,MMS11].

### **REACTION-DIFFUSION PROCESSES IN CATALYSIS AND RELATED SYSTEMS**

#### **CHEMISORPTION AND CATALYSIS ON METAL SURFACES [CR15 & PSS13 reviews]**

◆ Demonstration/analysis of metal-sulfur complex formation on metal surfaces [JCP16,JPCC16,..]

◆ First predictive molecular-level modeling of CO-oxidation on M(100) M = Pd, Rh,... under low-pressure (P) conditions including mixed adlayer ordering, realistic O<sub>2</sub> dissociation kinetics, CO steering, rapid diffusion, etc., obtaining ab-initio bifurcation diagrams, TPR spectra,... [JPCC16,CR15,PSS13]

◆ First realistic Onsager-type treatment of collective diffusion in mixed reactant systems as input to exact hydrodynamic reaction-diffusion equations; developed “equation-free heterogeneous multiscale method” preceding extensive development of HMM in 2000’s: our heterogeneous coupled lattice-gas (HCLG) simulation was applied for analysis of reaction fronts and patterns [CR15,PSS13,JCP06,MMS05,JCP95].

◆ Analyzed fluctuation-mediated behavior in nanoscale reaction systems, specifically noise-induced transitions in bistable and multistable systems [PSS13,JCMP07,PRL99].

#### **CATALYSIS IN NANOPOROUS SYSTEMS WITH INHIBITED DIFFUSIVE TRANSPORT**

◆ Generalized hydrodynamic formulation of interplay between inhibited transport (including single-file diffusion) and catalytic conversion reactions in nanoporous materials [JCP16,CR15,PRL12].

◆ Langevin and Fokker-Planck analysis of inhibited molecular passing in narrow pores [JCP18,PRL14].

◆ Catalytic polymerization reaction in nanopores: non-Markovian extrusion kinetics [JCP10].

#### **FUNDAMENTAL STATISTICAL MECHANICS OF NON-EQUILIBRIUM SYSTEMS**

◆ Discovery of generic two-phase coexistence in simple lattice-gas Schloegl type models with a discontinuous transition; analyzed metastability; developed nucleation theory [PRL18,JCP15,09,PRL07].

◆ Analysis of bistability and reaction front propagation, including precise determination of equistability, in the hydrodynamic limit (with rapid diffusion) for lattice-gas reaction-diffusion models [Chaos02]

◆ Non-equilibrium phase transitions: tricriticality [PA12], Ising vs MF criticality [JSP04], order-disorder transitions and percolative transport [PRL00], KPZ-type interface propagation [PRE94], correlated percolation [RMP93], epidemic analysis for discontinuous transitions to absorbing states [PRL91], etc.

◆ Random (and Cooperative) Sequential Adsorption (RSA) [RMP93].

**Top cited papers (numbering from publication list) with  $\geq 50$  cites (Web of Science 08/23):**

[R1] Evans, Rev. Mod. Phys. (1993) Random and Cooperative Sequential Adsorption.....	900
[R2] Evans et al., Surf. Sci. Reports (2006) Morphological Evolution in Thin Films.....	567
[72] Bartelt & Evans, PRB (1992) Scaling Analysis of Diffusion-mediated Island Growth.....	430
[93] Wen et al., PRL (1994) Diffusion of Large 2D Ag Clusters on Ag(100).....	285
[55] Evans et al., PRB (1990) Low-Temperature Epitaxial Growth.....	225
[100] Wen et al., PRL (1996) Coarsening Mechanisms in a Metal Film.....	179
[82] Bartelt & Evans, Surf. Sci. (1993) Nucleation and Growth of Square Islands.....	149
[102] Bartelt & Evans, PRB (1996) Exact Island Size Distributions for... Deposition.....	139
[87] Evans & Bartelt, JVSTA (1994) Nucleation and Growth in Metal... Homoepitaxy.....	133
[66] Evans, Langmuir (1991) Kinetic Phase Transitions in Catalytic Reaction Models.....	126
[97] Bartelt & Evans, PRL (1995) Transition to Multilayer Kinetic Roughening.....	119
[118] Suchorski et al., PRL (1999) Fluctuation-induced Transitions in a Bistable Reaction.....	117
[61] Evans & Miesch, PRL (1991) ...Kinetics of a First-Order Poisoning Transition.....	113
[R4] Liu et al. PSS (2015) Growth morphology and properties of metals on graphene.....	111
[60] Evans, PRB (1991) Factors mediating Smoothness in Epitaxial...Growth.....	107
[91] Gunther et al., PRL (1994) Anisotropy in Nucleation and Growth of 2D Islands.....	83
[185] Thiel et al. JPCC (2009) Coarsening of 2D Nanoclusters on surfaces.....	85
[11] Evans et al. JCP (1983) Irreversible Random and Cooperative Processes.....	85
[117] Bartelt et al, PRB (1999) Adatom Capture by Arrays of 2D Islands.....	76
[21] Nord & Evans, JCP (1985) Irreversible Random Immobile Adsorption.....	76
[113] Bartelt et al., PRL (1998) Island Size and Environment Dependence of Adatom Capture.....	74
[132] Suchorski et al., PRB (2001) Fluctuations & critical phenomena in catalytic CO-oxidation...72	72
[88] Bartelt & Evans, Surf. Sci. Lett. (1994) Dendritic Islands in Metal-on-Metal Epitaxy.....	66
[114] Stoldt et al., PRL (1998) Evolution of Far-From-Equilibrium Nanostructures.....	65
[62] Evans & Miesch, Surf. Sci. (1991) Catalytic Reaction Kinetics near...poisoning transition....	64
[95] Bartelt et al. Surf. Sci. Lett. (1995) Transitions in Critical Size for Metal(100) Homoepitaxy...64	64
[96] Tammaro et al., JCP (1995) Hybrid Treatment of Spatiotemporal Behavior in...Reactions.....	61
[79] Bartelt et al, PRB (1993) Island Size Scaling in Surface Deposition Processes.....	61
[xxx] Wei et al., ACS Catal. (2020) Hydrogenation of nitrate to ammonia w/o noble metals.....	60
[yyy] Han et al., Surf. Sci. (2019) Surface energies, adhesion,...Cu-graphite and Cu-graphene....	60
[99] Bartelt et al., PRB (1996) Island Size Distributions...influence of small cluster mobility.....	59
[129] Stoldt et al. PRL (2000) Using temperature to tune film roughness.....	59
[R5] Liu & Evans, Prog Surf Sci (2015) Multi-site LG modeling + KMC of surface reactions.....	57
[121] Stoldt et al. JCP (1999) Smoluchowski ripening of Ag islands on Ag(100).....	57
[146] Fournée et al. PRB (2003) Nucleation & growth of Ag films on a quasicrystalline surface.....	56
[140] Caspersen et al PRB (2002) Development & ordering of mounds in metal(100) homoepi.....	56
[162] Albao et al. PRB (2005) Monotonically decreasing size distributions: Ga rows on Si(100)...55	55
[111] Zhang et al Surf Sci (1998) Island formation and onset of multilayer growth Ag/Ag(100).....	56
[75] Evans, JCP (1993) ZGB surface reaction model with high diffusion rates.....	55
[81] Meng et al. PRE (1993) Kinetics and steady-state of A+BC surface reactions.....	54
[zzz] Appy et al, Prog. Surf. Sci. (2014) Transition metals on the (0001) surface of graphite.....	53
[92] Evans & Ray, PRE (1994) Interface propagation & nucleation for discontinuous transitions...53	53
[69] Kang & Evans, SS (1992) Scaling of surface roughness and Bragg oscillation decay.....	53
[46] Evans, PRB (1989) Random deposition models for thin film epitaxial growth.....	53
[131] Caspersen et al PRB (2001) Morphology of multilayer Ag/Ag(100) films vs deposition T....53	53
[159] Cox et al. PRB (2005) T-dependence of island growth shapes for Ag on Ag(111).....	53
[145] Evans et al PRB (2002) Island sizes and capture zone areas: JPD scaling & factorization.....	53
[134] Evans & Bartelt PRB (2001) Nucleation, adatom capture, island size distributions.....	52
[44] Chang et al. Surf. Sci. (1988) Oxygen-stabilized reconstructions of Pd(100).....	50
[49] Evans, PRL (1989) Kinetics of random sequential adsorption – comment.....	50
[aaa] Evans et al, Chaos (2002) From atomistic LG models for surface rxn to hydrodynamics.....	50
[bbb] Fournée et al, Surf. Sci. (2003) Growth of thin Ag films on quasicrystals and approx.....	50

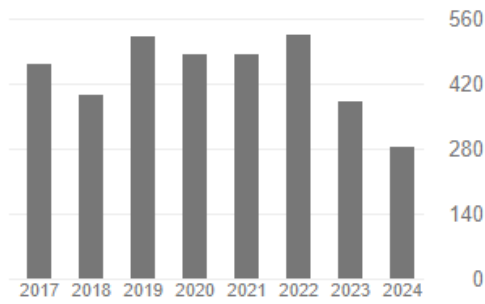
**PROFESSIONAL ACTIVITIES: SUMMARY OF PAPERS AND PUBLICATIONS**

<b>Date</b>	<b>Referred Publications in Print</b>	<b>Books/Chapters</b>	<b>Invited Papers/Talks</b>	<b>Contributed Papers</b>	<b>Citations (<i>Web of Science</i>)</b>
2024	6 to date	0/0	1	0	~180 to date
2023	9	0/0	3	1	299
2022	8	0/0	3	0	407
2021	10	0/0	3+1 cancelled	2	365
2020	15	0/1	1+ 6 cancelled	0	316
2019	12	0/0	2	1	385
2018	6	0/0	5	0	276
2017	6	0/0	6	1	342
2016	12	0/0	3	1	312
2015	10	0/0	3	0	388
2014	9	0/0	6	1	298
2013	8	0/0	5	2	275
2012	8	0/0	8	2	265
2011	12	0/0	4	5	352
2010	12	0/1	8	3	319
2009	13	0/0	14	2	303
2008	4	0/0	6	3	254
2007	9	0/1	3	5	360
2006	6	0/0	4	3	324
2005	9	0/1	10	4	269
2004	6	0/1	4	4	277
2003	8	0/0	4	5	307
2002	9	0/1	8	4	331
2001	6	0/0	6	2	303
2000	11	0/0	10	1	357
1999	7	0/1	4	2	293
1998	12	0/2	7	0	325
1997	3	0/1	6	2	302
1996	6	0/1	6	5	297
1995	5	0/0	8	1	214
1994	10	0/1	7	2	203
1993	13	0/0	8	2	213
1992	6	0/0	8	8	140
1991	10	0/0	5	4	101
1990	7	0/0	0	5	83
1989	8	0/0	0	3	72
1988	7	0/0	1	1	37
1987	7	0/0	0	1	53
1979-1986	2	0/1	3	15	135

**CITATIONS from GOOGLE SCHOLAR**

As of 08/2024: **Total cites  $\geq$  14,325; h-index = 58**

	All	Since 2019
Citations	14236	2684
h-index	58	23
i10-index	253	59

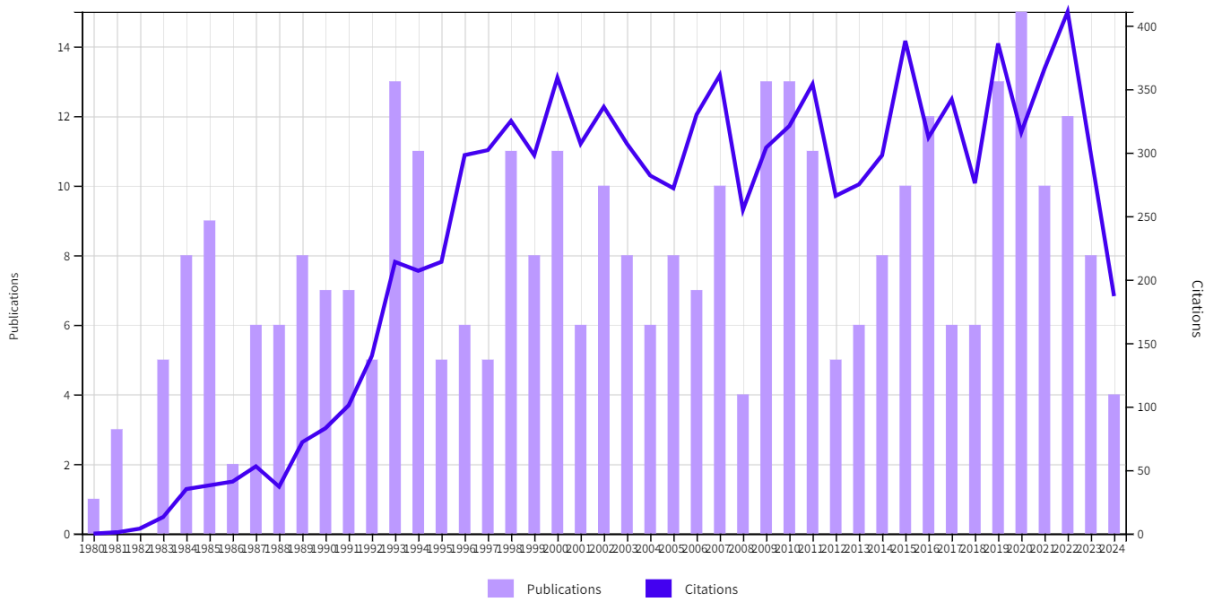


**CITATIONS from Clarivate WEB OF SCIENCE:**

As of 08/2024: **Total cites  $>$  10,385; h-index = 50.**

Times Cited and Publications Over Time

[DOWNLOAD](#)



**PAPERS AND PUBLICATIONS DETAILS****REFEREED JOURNAL PUBLICATIONS IN PRINT**

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).
10. 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).
11. 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  $j_z$ -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. Math. Phys.* 25, 2519-2526 (1984).
18. 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).
23. C. K. Chan, D. K. Hoffman and J. W. Evans, "Energy Sudden Dissociative Collisions: Structure & Applications of Factorization Relations," *J. Chem. Phys.* 82, 1855-1868 (1985).
24. J. W. Evans and R. S. Nord, "Competitive Irreversible One-, Two-, Three-, Point Adsorption on 2D Lattices," *Phys. Rev. B* 31, 1759-1769 (1985).
25. R. S. Nord, D. K. Hoffman and J. W. Evans, "Cluster Size Distributions for Irreversible Cooperative Filling of Lattices I: Exact 1D Results for Coalescing Clusters," *Phys. Rev. A* 31, 3820-3830 (1985).
26. J. W. Evans and R. S. Nord, "Cluster Size Distributions for Irreversible Cooperative Filling of Lattices II: Exact 1D Results for Non-Coalescing Clusters," *Phys. Rev. A* 31, 3831-3840 (1985).
27. C. K. Chan, D. K. Hoffman and J. W. Evans, "General Factorization Relations and Consistency Conditions in the Sudden Approximation via Infinite Matrix Inversion," *J. Chem. Phys.* 83, 1637-1647 (1985).
28. J. W. Evans, "Splitting Methods for Time-Independent Wave Propagation in Random Media," *J. Math. Phys.* 26, 2196-2200 (1985).
29. J. W. Evans and R. S. Nord, "Random Walks on Finite Lattices with Multiple Traps: Application to Particle-Cluster Aggregation," *Phys. Rev. A* 32, 2926-2943 (1985).
30. J. W. Evans, J. A. Bartz and D. E. Sanders, "Multi-Cluster Growth via Irreversible Cooperative Filling on Lattices," *Phys. Rev. A* 34, 1434-1448 (1986).
31. J. W. Evans, "Two-Hilbert Space Formulations of the Quantum Statistical Mechanics of Reactive Fluids: Dimer Formation and Decay," *J. Chem. Phys.* 85, 5991-6003 (1986).
32. J. W. Evans and R. S. Nord, "Diffraction from Disordered One-Dimensional Islands with Domain Boundaries: Intensity Behavior for Various Statistical Approximations," *Phys. Rev. B* 35, 6004-6016 (1987).
33. J. W. Evans and R. S. Nord, "Structure and Diffracted Intensity in a Model for Irreversible Island-Forming Chemisorption with Domain Boundaries," *J. Vac. Science Tech. A* 5, 1040-1044 (1987).
34. J. W. Evans, "Isomorphisms for Random Sequential Packing on Lattices," *J. Phys. A* 20, 3063-3069 (1987).
35. H. Pak and J. W. Evans, "Influence of Adlayer Statistics on Desorption Kinetics: Order-Disorder Effects," *Surface Science* 186, 550-562 (1987).
36. J. W. Evans "Non-Equilibrium Percolative  $c(2 \times 2)$  Ordering: Oxygen on Pd(100)," *J. Chem. Phys.* 87, 3038-3048 (1987).
37. J. W. Evans, "Correlated Percolation: Exact Bethe Lattice Analyses," *J. Phys. A* 20, 6487-6500 (1987).
38. J. W. Evans, D. K. Hoffman and H. Pak, "Desorption from an Immobile Adlayer: Exact One-Dimensional Kinetics," *Surface Science* 192, 475-490 (1987).
39. J. W. Evans, "Splitting Methods and Invariant Imbedding for Time-Independent Wave Propagation in Focusing Media and Waveguides," *J. Math. Phys.* 29, 97-102 (1988).

40. J. W. Evans, D. E. Sanders, "Percolative Aspects of Non-equilibrium Adlayer Structure," *J. Vac. Sci. Technol. A* 6, 726-729 (1988).
41. J. W. Evans, R. S. Nord and J. A. Rabaey, "Non-equilibrium  $c(2 \times 2)$  Island-Formation during Chemisorption: Scaling of Spatial Correlations and Diffracted Intensity," *Phys. Rev. B* 37, 8598-8611 (1988).
42. J. W. Evans and H. Pak, "Desorption from Non-Equilibrium Island-forming Adlayers," *Surface Science* 199, 28-42 (1988).
43. D. E. Sanders and J. W. Evans, "Correlated Percolation in Island-Forming Processes: Analysis of Cooperative Filling on a Square Lattice," *Phys. Rev. A* 38, 4186-4197 (1988).
44. S.-L. Chang, P. A. Thiel, J. W. Evans, "Oxygen-Stabilized Reconstructions of Pd(100): Phase Transitions during Oxygen Desorption," *Surface Science* 205, 117-142 (1988).
45. J. W. Evans and D. E. Sanders, "Percolative  $c(2 \times 2)$  Adlayer Structure in Non-equilibrium Adsorption Models," *Phys. Rev. B* 39, 1587-1594 (1989).
46. J. W. Evans, "Random Deposition Models for Thin Film Epitaxial Growth," *Phys. Rev. B* 39, 5655-5664 (1989).
47. J. W. Evans, "Relationship between Disordered  $c(2 \times 2)$  Structure and Diffracted Intensity: 5-Site Filling Model & Hard-Square Lattice Gas," *Surface Science* 215, 319-331 (1989).
48. D. K. Flynn, J. W. Evans and P. A. Thiel, "Temperature Dependence of Metal Film Growth via LEED Intensity Oscillations: Pt/Pd(100)," *J. Vac. Sci. Tech. A* 7, 2162-2166 (1989).
49. J. W. Evans, Comment on "Kinetics of Random Sequential Adsorption," *Phys. Rev. Lett.* 62, 2642 (1989).
50. J. W. Evans, "Analysis of a Diffusion-Limited Island Growth Mechanism for Chemisorption and Epitaxy," *Phys. Rev. A (Rapid Comm.)* 40, 2868-2870 (1989).
51. J. W. Evans and C. A. Hurst, "Cooperative Adsorption-Desorption Models with Random Steady States," *Phys. Rev. A (Rapid Communication)* 40, 3461-3463 (1989).
52. J. W. Evans, D. K. Flynn and P. A. Thiel, "Influence of Adsorption-Site Geometry and Diffusion on Thin-Film Growth: Pt/Pd(100)," *Ultramicroscopy*, 31, 80-86 (1989).
53. J. W. Evans, "Diffusion of Non-interacting Particles into a Semi-Infinite Lattice," *Phys. Rev. B* 41, 2158-2162 (1990).
54. J. W. Evans, "Modeling of Epitaxial Thin-Film Growth on fcc(100) Substrates at Low-Temperature," *Vacuum* 41, 479-481 (1990). (Proc. ICSOS 7 & 11th IVC, Köln 1989)
55. J. W. Evans, D. E. Sanders, P. A. Thiel and A. E. DePristo, "Low-Temperature Epitaxial Growth of Thin Film Metal Films," *Phys. Rev. B. (Rapid Comm.)* 41, 5410-5413 (1990).
56. J. W. Evans, "From Lattice to Continuum Percolation via Clustering," *J. Phys. A* 23, L197-L200 (1990).
57. J. W. Evans, "Irreversible Processes with Nearest-Particle Rates," *J. Phys. A* 23, 2227-2230 (1990).
58. R. S. Nord and J. W. Evans, "Inequivalent Models of Irreversible Dimer Filling: 'Transition State' Dependence," *J. Chem. Phys.* 93, 8397-8398 (1990).
59. H. C. Kang, P. A. Thiel and J. W. Evans, "Cluster Diffusivity: Structure, Correlation and Scaling," *J. Chem. Phys.* 93, 9018-9025 (1990).
60. J. W. Evans, "Factors Mediating Smoothness in Epitaxial Thin-Film Growth," *Phys. Rev. B* 43, 3897-3905 (1991).

61. J. W. Evans and M. S. Miesch, "Characterizing Kinetics below a First-Order Catalytic Poisoning Transition," *Phys. Rev. Lett.* 66, 833-836 (1991).
62. J. W. Evans and M. S. Miesch, "Catalytic Reaction Kinetics near a First-Order Poisoning Transition," *Surface Science* 245, 401-410 (1991).
63. H. C. Kang, D. K. Flynn-Sanders, P. A. Thiel and J. W. Evans, "Diffraction Profile Analysis for Epitaxial Growth on FCC(100) Substrates: Diffusionless Models," *Surface Sci.*, 256, 205-215 (1991).
64. H. C. Kang and J. W. Evans, "Scaling Behavior of Deposition Models with Limited Downward Mobility," *Phys. Rev. A* 44 2335-2344 (1991).
65. J. W. Evans and H. C. Kang, "Analytic Observations for the  $d=1+1$  Bridge Site (or Single-Step) Deposition Model," *J. Math. Phys.* 32, 2918-2922 (1991).
66. J. W. Evans, "Kinetic Phase Transitions in Catalytic Reaction Models," *Langmuir*, 7, 2514-2519 (1991).
67. H. C. Kang and J. W. Evans, "Scaling Analysis of Surface Roughness for Simple Models of Molecular-Beam Epitaxy," *Surface Science*, 269-270, 784-789 (1992).
68. J. W. Evans, H. H. Madden and R. Imbihl, "Modelling Spatio-temporal Behavior of the NO + CO Reaction on Pt," *J. Chem. Phys. (Communication)*, 96, 4805-4807 (1992).
69. H. C. Kang and J. W. Evans, "Scaling Analysis of Surface Roughness and Bragg Oscillation Decay in Models for Low-Temperature Epitaxial Growth," *Surface Science*, 271, 321-330 (1992).
70. J. W. Evans, "Kinetic Phase Diagrams for the Monomer-Dimer Surface Reaction: Unification of Mean-Field and Lattice-Gas Behavior," *J. Chem. Phys.*, 97, 572-577 (1992).
71. J. W. Evans and R. S. Nord, "Random and Cooperative Sequential Adsorption on Infinite Ladders and Strips," *J. Stat. Phys.*, 69, 151-162 (1992).
72. M. C. Bartelt and J. W. Evans, "Scaling Analysis of Diffusion-mediated Island Growth in Surface Adsorption Processes," *Phys. Rev. B.*, 46, 12675-12687 (1992).
73. M. C. Bartelt and J. W. Evans, "Crossover from Anisotropic to Isotropic Diffusion-Mediated Island Growth on Surfaces," *Europhys. Lett.*, 21, 99-103 (1993).
74. J. W. Evans and T. R. Ray, "Kinetics of the Monomer-Monomer Surface Reaction Model," *Phys. Rev. E*, 47, 1018-1025 (1993).
75. J. W. Evans, "ZGB Surface Reaction Model with High Diffusion Rates," *J. Chem. Phys.*, 98, 2463-2465 (1993).
76. J. W. Evans, M. C. Bartelt, "Irreversible Island Formation during Deposition: Separation Distributions and Diffraction Profiles," *Surface Science.*, 284 L437-443 (1993).
77. M. C. Bartelt and J. W. Evans, "Initial Evolution of Kashchiev Models of Thin-Film Growth," *J. Phys. A*, 26, 2743-2754 (1993).
78. D. K. Flynn-Sanders, J. W. Evans, and P. A. Thiel, "Homoepitaxial Growth on Pd(100)," *Surface Science*, 289, 75-84 (1993).
79. M. C. Bartelt, M. C. Tringides and J. W. Evans, "Island-Size Scaling in Surface Deposition Processes," *Phys. Rev. B.*, 47, 13891-13894 (1993).
80. M. C. Bartelt, J. W. Evans, M. C. Glasser, "The Car-Parking Limit of Random Sequential Adsorption: Expansions in One Dimension," *J. Chem Phys.*, 99, 1438-1439 (1993).
81. B. Meng, W. H. Weinberg, J. W. Evans, "Transitions in the Kinetics and Steady States of Irreversible A+BC Surface Reaction Models," *Phys. Rev. E.*, 48, 3577-3588 (1993).

82. M. C. Bartelt, J. W. Evans, "Nucleation and Growth of Square Islands during Deposition: Sizes, Coalescence, Separations & Correlations," *Surface Science*, 298, 421-431 (1993).
83. J. W. Evans, D. K. Flynn-Sanders and P. A. Thiel, "Surface Self-Diffusion Barrier for Pd(100) from Low-Energy-Electron-Diffraction," *Surface Science*, 298, 378-383 (1993).
84. J. W. Evans and M. C. Bartelt, "Kinetics of Restricted Solid-on-Solid Models of Film Growth," *Phys. Rev. E.*, 49, 1061-1069 (1994).
85. W. Swiech, C. S. Rastomjee, R. Imbihl, J. W. Evans, B. Rausenberger, W. Engel, A. K. Schmid, A. M. Bradshaw, and E. Zeitler, "On the Complex Structure of Reaction-Diffusion Fronts Observed During CO-oxidation on Pt{100}," *Surface Sci.*, 307/309, 138-142 (1994).
86. M. C. Bartelt and J. W. Evans, "Scaling of Spatial Correlations for Cooperative Sequential Adsorption with Clustering," *J. Stat. Phys.*, 76, 867-876 (1994).
87. J. W. Evans and M. C. Bartelt, "Nucleation and Growth in Metal-on-Metal Homoepitaxy: Rate Equations, Simulations and Experiments," *J. Vac. Sci. Technol. A* 12, 1800-1808 (1994).
88. M. C. Bartelt and J. W. Evans, "Dendritic Islands in Metal-on-Metal Epitaxy I: Shape Transitions and Diffusion at Island Edges," *Surface Science*, 314, L829-834 (1994).
89. M. C. Bartelt and J. W. Evans, "Dendritic Islands in Metal-on-Metal Epitaxy II: Coalescence and Multilayer Growth," *Surface Science*, 314, L835-842 (1994).
90. B. Meng, W. H. Weinberg, and J. W. Evans, "Lattice-Gas Model mimicking the NO + CO Reaction in Pt(100)," *J. Chem. Phys.*, 101, 3234-3242 (1994).
91. S. Gunther, E. Kopatzki, M. C. Bartelt, J. W. Evans, and R. J. Behm, "Anisotropy in Nucleation and Growth of Two-Dimensional Islands during Homoepitaxy on 'Hex' Reconstructed Au(100)," *Phys. Rev. Lett.*, 73, 553-556 (1994).
92. J. W. Evans and T. R. Ray, "Interface Propagation and Nucleation Phenomena for Discontinuous Poisoning Transitions in Surface Reaction Models," *Phys. Rev. E.*, 50, 4302-4314 (1994).
93. J.-M. Wen, S.-L. Chang, J. W. Burnett, J. W. Evans, and P. A. Thiel, "Diffusion of Large Two-Dimensional Ag Clusters on Ag(100)," *Phys. Rev. Lett.*, 73, 2591-2594 (1994).
94. M. Tammaro and J. W. Evans, "Monomer-dimer Surface Reaction Model: Influence of the Dimer Adsorption Mechanism", *Phys. Rev. E*, 52, 2310-2317 (1995).
95. M. C. Bartelt, L. S. Perkins, and J. W. Evans, "Transitions in the Critical Size for Metal(100) Homoepitaxy", *Surface Science*, 344, L1193-1199 (1995).
96. M. Tammaro, M. Sabella, and J. W. Evans, "Hybrid Treatment of Spatio-Temporal Behavior in Surface Reactions with Coexisting Immobile and Highly Mobile Reactants", *J. Chem. Phys.* 103, 10277-10285 (1995).
97. M. C. Bartelt and J. W. Evans, "Transition to Multilayer Kinetic Roughening for Metal(100) Homoepitaxy", *Phys. Rev. Lett.*, 75, 4250-4253 (1995).
98. J. W. Evans and M. C. Bartelt, "Nucleation, Growth, and Kinetic Roughening of Metal (100) Homoepitaxial Thin Films", *Langmuir* 12, 217-229 (1996).
99. M. C. Bartelt, S. Gunter, E. Kopatzki, R. J. Behm, and J. W. Evans, "Island Size Distributions in Submonolayer Epitaxial Growth: Influence of the Mobility of Small Clusters", *Phys. Rev. B* 53, 4099-4104 (1996).
100. J.-M. Wen, J. W. Evans, M. C. Bartelt, J. W. Burnett, and P. A. Thiel, "Coarsening Mechanisms in a Metal Film: From Cluster Diffusion to Vacancy Ripening", *Phys. Rev. Lett.* 76, 652-655 (1996).
101. M. Tammaro and J.W. Evans, "Percolative Diffusion of CO during CO-Oxidation on Pt(100)", *J. Chem. Phys.* 104, 3386-3390 (1996).

- 102.** M.C. Bartelt and J.W. Evans, "Exact Island Size Distributions for Submonolayer Deposition: Influence of Correlations between Island Size & Separation", *Phys. Rev. B (Rapid Communication)* **54**, R17359-17362 (1996).
- 103.** C.-M. Zhang, M.C. Bartelt, J.-M. Wen, C.J. Jenks, J.W. Evans, and P.A. Thiel, "Initial Stages of Ag/Ag(100) Homoepitaxy: Scanning Tunneling Microscopy Experiments and Monte-Carlo Simulations", *J. Crystal Growth*, **174**, 851-857 (1997).
- 104.** Y. Li, M. C. Bartelt, J. W. Evans, N. Waelchli, E. Kamshoff, and K. Kern, "Transition from 1D to 2D Island Growth on Metal(110) Surfaces induced by Anisotropic Corner Rounding", *Phys. Rev. B*, **56**, 12539-12543 (1997).
- 105.** M. Tammaro and J. W. Evans, "Chemical Diffusivity and Wave Propagation in Surface Reactions: Lattice-Gas Model mimicking CO-Oxidation with High CO-Mobility", *J. Chem. Phys.* **108**, 762-773 (1998).
- 106.** M. Tammaro and J.W. Evans, "Chemical Diffusion in Mixed Adlayers and Wave Propagation in Surface Reactions", *Surface Science Letters*, **395** L207-214 (1998).
- 107.** L. Bardotti, M.C. Bartelt, C.J. Jenks, C.R. Stoldt, J.-M. Wen, C.-M. Zhang, P.A. Thiel and J.W. Evans, "Formation and Equilibration of Submonolayer Island Distributions in Ag/Ag(100) Homoepitaxy", *Langmuir*, **14**, 1487-1486 (1998).
- 108.** M. Tammaro and J.W. Evans, "Reactive Removal of Unstable NO+CO Adlayers: Chemical Diffusion and Reaction Front Propagation", *J. Chem. Phys.*, **108**, 7795-7806 (1998).
- 109.** M. Tammaro and J.W. Evans, "Hydrodynamic Limits for the Monomer-Dimer Surface Reaction Models: Chemical Diffusion, Wave Propagation, Equistability", *Phys. Rev. E*, **57**, 5087-5094 (1998).
- 110.** L. Bardotti, C.R. Stoldt, C.J. Jenks, M.C. Bartelt, J.W. Evans, and P.A. Thiel, "HRLEED Profile Analysis and Diffusion Barrier Estimation for Submonolayer Ag/Ag(100) Homoepitaxy", *Phys. Rev. B*, **57**, 12544-12549 (1998).
- 111.** C.-M. Zhang, M.C. Bartelt, J.-M. Wen, C.J. Jenks, J.W. Evans, and P.A. Thiel, "Submonolayer Island Formation and the Onset of Multilayer Growth during Ag/Ag(100) Homoepitaxy", *Surface Science*, **406**, 178-193 (1998).
- 112.** M. Tammaro, J.W. Evans, C.S. Rastomjee, W. Swiech, A.M. Bradshaw, and R. Imbihl, "Reaction-Diffusion Front Propagation across Stepped Surfaces during Catalytic Oxidation of CO on Pt(100)", *Surface Science*, **407**, 162-170 (1998).
- 113.** M.C. Bartelt, A.K. Schmid, J.W. Evans, and R.Q. Hwang, "Island Size and Environment Dependence of Adatom Capture: Cu/Co Islands on Ru(0001)", *Physical Review Letters* **81**, 1901-1904 (1998).
- 114.** C.R. Stoldt, A.M. Cadilhe, C.J. Jenks, J.-M. Wen, J.W. Evans, and P.A. Thiel, "Evolution of Far-From-Equilibrium Nanostructures Formed by Cluster-Step and Cluster-Cluster Coalescence in Metal Films", *Physical Review Letters* **81**, 2950-2953 (1998).
- 115.** C.R. Stoldt, A.M. Cadilhe, M.C. Bartelt, C.J. Jenks, P.A. Thiel, and J.W. Evans, "Formation and Relaxation of 2D Island Arrays in Metal(100) Homoepitaxy", *Prog. Surf. Sci.*, **59**, 67-77 (1998).
- 116.** J.R. Sanchez and J.W. Evans, "Diffusion of Small Clusters on Metal(100) Surfaces: Exact Master Equation Analysis", *Phys. Rev. B* **59**, 3224-3233 (1999).
- 117.** M.C. Bartelt, C.R. Stoldt, C.J. Jenks, P.A. Thiel, J.W. Evans, "Adatom Capture by Arrays of Two-Dimensional Ag Islands on Ag(100)", *Phys. Rev. B* **59**, 3125-3134 (1999).
- 118.** Yu. Suchorski, J. Beben, E.W. James, J.W. Evans, and R. Imbihl, "Fluctuation-Induced Transitions in a Bistable Surface Reaction: catalytic CO-oxidation on a Pt Field Emitter Tip", *Physical Review Letters*, **82**, 1907-1910 (1999).

119. M.C. Bartelt and J.W. Evans, "Temperature Dependence of Roughening during Metal(100) Homoepitaxy: Kinetic Phase Transition from Mounding to Smooth Growth", *Surface Science*, 423, 189-207 (1999).
120. A.M. Dabiran, S.M. Seutter, S. Stoyanov, M.C. Bartelt, J.W. Evans, and P.I. Cohen, "Step Edge Barriers vs Step Edge Relaxation in GaAs:Sn MBE", *Surface Science*, 438, 131-141 (1999).
121. C.R. Stoldt, C.J. Jenks, P.A. Thiel, A.M. Cadilhe, and J.W. Evans, "Smoluchowski Ripening of Ag Islands on Ag(100)", *J. Chem. Phys.*, 111, 5157-5166 (1999).
122. E.W. James, C. Song, J.W. Evans, "CO-Oxidation Model with Superlattice Ordering of Adsorbed Oxygen I. Steady-State Bifurcations", *J. Chem. Phys.*, 111, 6579-6589 (1999).
123. D.-J. Liu, J.W. Evans, Symmetry-Breaking and Percolation Transitions in a Surface Reaction Model with Superlattice Ordering, *Phys. Rev. Letters*, 84, 955-958 (2000).
124. A.M. Cadilhe, C.R. Stoldt, C.J. Jenks, P.A. Thiel, and J.W. Evans, "Evolution of Far-From-Equilibrium Nanostructures on Ag(100) Surfaces: Protrusions and Indentations at Extended Step Edges", *Phys. Rev. B* 61, 4910-4925 (2000).
125. P.A. Thiel and J.W. Evans, "Nucleation, Growth, and Relaxation of Thin Films in Metal(100) Homoepitaxy", *J. Phys. Chem. B* 104, 1663-1676 (2000) - Feature Article.
126. E.W. James, D.-J. Liu, and J.W. Evans, "Relaxation Effects in Random Sequential Adsorption: Application to Chemisorption Systems", *J. Colloids and Surfaces A*, 165, 241-254 (2000). (Special Issue: "Adhesion of Submicron Particles on Solid Surfaces", edited by V. Privman.)
127. M.C. Bartelt, J.B. Hannon, A.K. Schmid, C.R. Stoldt, and J.W. Evans, "Island Formation during Deposition and Etching", *J. Colloids and Surfaces A*, 165, 373-403 (2000). (ibid)
128. D.-J. Liu and J.W. Evans, "Ordering and Percolation Transitions for Hard-Squares: Equilibrium versus Non-equilibrium Models for Adsorbed Layers with  $c(2 \times 2)$  Superlattice Ordering", *Phys. Rev. B* 62, 2134-2145 (2000).
129. C.R. Stoldt, K.J. Caspersen, M.C. Bartelt, C.J. Jenks, J.W. Evans, and P.A. Thiel, "Using Temperature to Tune Film Roughness: Non-Intuitive Behavior in a Simple System", *Physical Review Letters*, 85, 800-803 (2000).
130. D.-J. Liu and J.W. Evans, "Surface Diffusion in Mixed Adlayers with Superlattice Ordering: Percolative Transport around Obstacles and along Domain Boundaries", *J. Chem. Phys.* 113, 10252-10264 (2000).
131. K.J. Caspersen, C.R. Stoldt, A.R. Layson, M.C. Bartelt, P.A. Thiel, and J.W. Evans, "Morphology of Multilayer Ag/Ag(100) Films versus Deposition Temperature: STM Analysis and Atomistic Lattice-Gas Modeling", *Phys. Rev. B*, 63, 085401 (2001), 15pp.
132. Yu. Suchorski, J. Beben, R. Imbihl, E.W. James, Da-Jiang Liu, and J.W. Evans, "Fluctuations and Critical Phenomena in Catalytic CO-Oxidation on Nanoscale Pt Facets", *Phys. Rev. B* 63, 165417 (2001), 12pp.
133. W.W. Pai, J.F. Wendelken, C.R. Stoldt, P.A. Thiel, J.W. Evans, and D.-J. Liu, "Evolution of Two-Dimensional Worm-Like Nanoclusters on Metal Surfaces", *Physical Review Letters* 86, 3088-3091 (2001).
134. J.W. Evans and M.C. Bartelt, "Nucleation, Adatom Capture, and Island Size Distributions: Unified Scaling Analysis for Submonolayer Deposition", *Phys. Rev. B*, 63, 235408 (2001), 15 pp.
135. K.J. Caspersen and J.W. Evans, "Homoepitaxial Growth of Metal Films at Very Low Temperatures: Lattice-Gas Models with Restricted Downward Funneling", *Phys. Rev. B*, 64, 075401 (2001), 11pp.

136. D.-J. Liu and J.W. Evans, "Phase Transitions in Mixed Adsorbed Layers: Effect of Repulsions between "Hard-Squares" and "Point-Particles" ", *J. Chem. Phys.*, 114, 10977-10978 (2001).
137. N. Pavlenko, J.W. Evans, D.-J. Liu, and R. Imbihl, "Catalytic CO Oxidation on Nanoscale Pt Facets: Effect of Inter-facet CO Diffusion on Bifurcation and Fluctuation Behavior", *Phys. Rev. E* 65, 016121 (2002), 8 pp.
138. J.W. Evans, D.-J. Liu, M. Tammaro, "From Atomistic Lattice-Gas Models for Surface Reactions to Hydrodynamic Reaction-Diffusion Equations", *Chaos* 12,131-143 (2002). (Invited Contribution for Focus Issue: Nonlinear Pattern Formation in Surface Science, edited by A.S. Mikhailov and G. Ertl)
139. A.R. Layson, J.W. Evans, and P.A. Thiel, "Additive-Enhanced Coarsening and Smoothing of Metal Films: Complex Mass-Flow Dynamics underlying Nanostructure Evolution", *Phys. Rev. B* 65, 193409 (2002), 4 pp. Also in *Virtual Journal of Nanoscale Science and Technology*, May 27, 2002.
140. K.J. Caspersen, A.R. Layson, C.R. Stoldt, V. Fournee, P.A. Thiel, and J.W. Evans, "Development and Ordering of Mounds during Metal(100) Homoepitaxy", *Phys. Rev. B* 65, 193407 (2002), 4pp.
141. C.H. Choi, D.-J. Liu, J.W. Evans, and M.S. Gordon, "Passive and Active Oxidation of Si(100) by Atomic Oxygen: Theoretical Study of Possible Reaction Mechanisms", *J. Am. Chem. Soc.* 124, 8730-8740 (2002).
142. D.-J. Liu and J.W. Evans, "Fluctuations and Bistability in a Hybrid Atomistic Model for CO Oxidation on Nanofacets: An Effective Potential Analysis", *J. Chem. Phys.* 117, 7319-7328 (2002).
143. D.-J. Liu and J.W. Evans, "Sintering of 2D Nanoclusters in Metal(100) Homoepitaxial Systems: Deviations from Predictions of Mullins Continuum Theory", *Phys. Rev. B.* 66, 165407 (2002), 12pp. Also in *Virtual J. of Nanoscale Science and Technology*, Oct.21, 2002.
144. S. Frank, H. Wedler, R.J. Behm, J. Rottler, P. Maass, K.J. Caspersen, C.R. Stoldt, P.A. Thiel, and J.W. Evans, "Approaching the Low Temperature Limit in Nucleation and Growth of fcc(100) Metal Films - Ag/Ag(100), *Phys. Rev. B* 66, 155435 (2002), 7pp.
145. J.W. Evans and M.C. Bartelt, "Island Sizes and Capture Zone Areas in Submonolayer Deposition: Analysis via Scaling and Factorization of the Joint Probability Distribution", *Phys. Rev. B* 66, 235410 (2002), 12pp.
146. V. Fournee, T.C. Cai, A.R. Ross, T.A. Lograsso, J.W. Evans, and P.A. Thiel, "Nucleation and Growth of Ag Films on a Quasicrystalline AlPdMn Surface", *Phys. Rev. B* 67, 033406 (2003), 4pp.
147. A.R. Layson, J.W. Evans, and P.A. Thiel, "The effect of common gases on nucleation of metal islands: The role of oxygen in Ag(100) homoepitaxy", *J. Chem. Phys.* 118, 6467-6472 (2003).
148. M. Li, M.C. Bartelt, and J.W. Evans, "Geometry-based Simulation of Submonolayer Film Growth", *Phys. Rev. B* 68, 121401(R) (2003), 4pp.
149. V. Fournee, A.R. Ross, T.A. Lograsso, J.W. Evans, and P.A. Thiel, "Growth of Ag Thin Films on Complex Surfaces of Quasicrystals and Approximant Phases", *Surface Science* 537, 5-26 (2003).
150. N. Pavlenko, R. Imbihl, J.W. Evans, and D.-J. Liu, "Critical Behavior in an Atomistic Surface Reaction Model exhibiting Bistability: CO-Oxidation with Rapid CO-diffusion", *Phys. Rev. E* 68, 016212 (2003), 8pp.
151. M. Li and J.W. Evans, "Geometry-based Simulation (GBS) Algorithms for Island Nucleation and Growth during Submonolayer Deposition", *Surface Science*, 546, 127-148 (2003).
152. M. Li and J.W. Evans, "Growth Coalescence Shapes for Islands during Metal(100) Homoepitaxy", *Phys. Rev. B* 69, 035410 (2004), 14pp.
153. D.-J. Liu, N. Pavlenko, and J.W. Evans, "Crossover between Mean-Field and Ising Critical Behavior in a Lattice-Gas Reaction-Diffusion Model", *J. Stat. Phys.*, 114, 101-114 (2004).

154. M.A. Albao, Da-Jiang Liu, C.H. Choi, M.S. Gordon, and J.W. Evans, "Atomistic Modeling of Morphological Evolution during Simultaneous Etching and Oxidation of Si(100)", *Surface Science*, 555, 51-67 (2004).
155. P.A. Thiel and J.W. Evans, "Energetic Parameters for Atomic Scale Processes on Ag(100)", *J. Phys. Chem. B* 108, 14428-14433 (2004) (Invited for Special Issue commemorating Gerhardt Ertl).
156. D.-J. Liu and J.W. Evans, "Lattice-Gas modeling of the formation and ordering of oxygen adlayers on Pd(100)", *Surface Science* 563, 13-26 (2004).
157. D.-J. Liu and J.W. Evans, "From Atomic Scale Reactant Ordering to Mesoscale Reaction Front Propagation: CO Oxidation on Pd(100)", *Phys. Rev. B* 70, 193408 (2004), 4pp.
158. M. Li and J.W. Evans, "Modeling of Island Formation during Submonolayer Deposition: A Stochastic Geometry-Based Simulation (GBS) Approach", *SIAM Multiscale Modeling & Simulation* 3, 629-657 (2005).
159. E. Cox, M. Li, P.-W. Chung, C. Ghosh, T.S. Rahman, C.J. Jenks, J.W. Evans, and P.A. Thiel, "Temperature-dependence of island growth shapes in submonolayer deposition of Ag on Ag(111)", *Phys. Rev. B* 71, 115414 (2005), 9pp.
160. J. Ledieu, R. McGrath, N.V. Richardson, Q. Chen, V. Fournee, T. Lograsso, A. Ross, K.J. Caspersen, U. Baris, J.W. Evans, and P.A. Thiel, "Step Structure on the Five-Fold Al-Pd-Mn Quasicrystalline Surface and on Related Surfaces", *Surf. Sci.* 583, 4-15 (2005).
161. D.-J. Liu and J.W. Evans, "From Atomic Scale Ordering to Mesoscale Spatial Patterns in Surface Reactions: A Heterogeneous Coupled Lattice-Gas (HCLG) Simulation Approach", *SIAM Multiscale Modeling & Simulation* 4, 424-446 (2005).
162. M.A. Albao, M.M.R. Evans, J. Nogami, D. Zorn, M.S. Gordon, and J.W. Evans, "Monotonically decreasing size distributions for one-dimensional Ga rows on Si(100)", *Phys. Rev. B* 72, 035426 (2005), 8pp. Also listed in *Virtual Journal of Nanoscale Science and Technology*, 2005.
163. M.A. Albao, D.-J. Liu, M.S. Gordon, and J.W. Evans, "Simultaneous etching and oxidation of vicinal Si(100) surfaces: Atomistic lattice-gas modeling of morphological evolution", *Phys. Rev. B* 72, 195420 (2005), 12pp.
164. M. Li and J.W. Evans, "Theoretical analysis of mound slope selection during unstable multilayer growth", *Phys. Rev. Lett.* 95, 256101 (2005), 4pp; 96, 079902(E) (2006), 1pp.
165. C. Ghosh, D.-J. Liu, C.J. Jenks, P.A. Thiel, and J.W. Evans, "Modeling of the energetics and kinetics of Al-deposition on 5-fold Al-rich quasicrystal surfaces", *Phil. Mag.*, 86, 831-840 (2006).
166. M. Li and J.W. Evans, "Mound Slope and Shape Selection during Unstable Multilayer Growth: Analysis of Step Dynamics Model including Downward Funneling", *Phys. Rev. B*, 73, 125434 (2006), 13pp.
167. C. Ghosh, D.-J. Liu, K.J. Schnitzenbaumer, C.J. Jenks, P.A. Thiel, and J.W. Evans, "Island formation during Al deposition on 5-fold Al-Cu-Fe quasicrystalline surfaces: Kinetic Monte Carlo simulation of a disordered-bond-network lattice-gas model", *Surf. Sci.*, 600, 2220-2230 (2006).
168. D.-J. Liu and J.W. Evans, "Atomistic lattice-gas modeling of CO-oxidation on Pd(100): Temperature-programmed spectroscopy and steady-state behavior", *J. Chem. Phys.*, 124, 154705 (2006), 13pp.
169. D.-J. Liu and J.W. Evans, "Chemical diffusion in mixed CO+O adlayers and reaction front propagation in CO-oxidation on Pd(100)", *J. Chem. Phys.*, 125, 054709 (2006), 8pp.



170. M.A. Albao, M.M.R. Evans, J. Nogami, D. Zorn, M.S. Gordon, and J.W. Evans, "Reply to Comment on "Monotonically decreasing size distributions for one-dimensional Ga rows on Si(100)", Phys. Rev. B, 74, 037402 (2006), 3pp.
171. D.-J. Liu, X. Guo, and J.W. Evans, "Quadratic Contact Process: Phase Separation with Interface-Orientation-Dependent Equistability", Phys. Rev. Lett. 98, 050601 (2007), 4pp.
172. D.-J. Liu and J.W. Evans, Fluctuations and patterns in nanoscale surface reaction systems: Influence of reactant phase separation during CO oxidation", Phys. Rev. B 75, 073401 (2007), 4pp.
173. D.-J. Liu and J.W. Evans, Fronts and fluctuations in a tailored model for CO oxidation on metal(100) surfaces", submitted to J. Phys.: Cond. Matt. 19, 065129 (2007), 14pp. (Special issue on *Chemical kinetics beyond the textbook*, K. Lindenberg, G. Oshanin, and M. Tachiya, ed.s)
174. B. Unal, J.W. Evans, T.A. Lograsso, A.R. Ross, C.J. Jenks, and P.A. Thiel, "Terrace-dependent Nucleation of Small Ag Clusters on a Five-fold Icosahedral Quasicrystal Surface", Phil. Mag., 87, 2995-3001 (2007).
175. B. Unal, A.R. Ross, T.A. Lograsso, K.J. Schnitzenbaumer, C. Ghosh, C.J. Jenks, J.W. Evans, and P.A. Thiel, "Nucleation of Ag thin films on five-fold surfaces of i-Al-Pd-Mn quasicrystals", Phys. Rev. B, 75, 064205 (2007), 9pp.
176. M. Shen, J.M. Wen, C.J. Jenks, P.A. Thiel, D.-J. Liu, and J.W. Evans, "Ripening of monolayer vacancy pits on metal surfaces: Pathways, energetics, and size-scaling for Ag(111) versus Ag(100)", Phys. Rev. B, 75 (2007) 245409, 10pp.
177. X. Guo, D.-J. Liu, and J.W. Evans, "Generic Two-phase Coexistence, Relaxation Kinetics, and Interface Propagation in the Quadratic Contact Process: Simulation Studies", Phys. Rev. E 75, 061129 (2007), 13 pp.
178. B. Unal, F. Qin, Y. Han, D.-J. Liu, D. Jing, A.R. Layson, C.J. Jenks, J.W. Evans, and P.A. Thiel, "Scanning Tunneling Microscopy and Density Functional Theory Study of Initial Bilayer Growth of Ag Films on NiAl(110)", Phys. Rev. B, 76, 195410 (2007), 11pp.
179. M. Li, J.W. Evans, C.Z. Wang, M. Hupalo, M.C. Tringides, T.-L. Chan, and K.M. Ho, "Strongly Driven Coarsening of Height-Selected Pb Islands on Si(111), Surf. Sci. Lett., 601, L140-144 (2007).
180. Y. Han, D.-J. Liu, B. Unal, F. Qin, D. Jing, C.J. Jenks, P.A. Thiel, and J.W. Evans, "Kinetics of Facile Bilayer Island Formation for Ag on NiAl(110)", Phys. Rev. Lett., 100, 116105 (2008).
181. M. Li, P.-W. Chung, E. Cox, C.J. Jenks, P.A. Thiel, and J.W. Evans, "Exploration of Complex Multilayer Film Growth Morphologies: STM Analysis and Predictive Atomistic Modeling for Ag on Ag(111), Phys. Rev. B, 77, 033402 (2008), 4pp.
182. X. Guo, J.W. Evans, and D.-J. Liu, "Generic Two-phase Coexistence, Relaxation Kinetics, and Interface Propagation in the Quadratic Contact Process: Analytic Studies", Physica A 387, 177-201 (2008).
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, 602, 2532-2540 (2008).
184. B. 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 & Step Dynamics Modeling", Physical Review Letters, 102, 196103 (2009), 4pp.
185. P.A. Thiel, M. Shen, D.-J. Liu and J.W. Evans, "Coarsening of two-dimensional nanoclusters on metal surfaces", J. Phys. Chem. C (Invited Centennial Feature Article), 113, 5047-5067 (2009).
186. 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 Issue in honor of Gerhard Ertl 2007 Nobel Laureate in Chemistry), 603, 1706-1716 (2009).

- 187.** M. Shen, D.-J. Liu, C.J. Jenks, J.W. Evans, and P.A. Thiel, “The effect of chalcogens (O,S) on coarsening of nanoislands on metal surfaces” *Surf. Sci.* (Invited for Ertl Issue), 603, 1486-1491 (2009).
- 188.** 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*, 517, 1949-1957 (2009).
- 189.** M. Li, Y. Han, P.A. Thiel, and J.W. Evans, “Formation of complex wedding-cake-like morphologies during homoepitaxial growth of Ag on Ag(111): Atomistic, step-dynamics, and continuum modeling”, *J. Phys. Cond. Matt.* (Invited for Special Issue), 21, 084216 (2009).
- 190.** X. Guo, D.-J. Liu, and J.W. Evans, “Schloegl’s Second Model for Autocatalysis with Particle Diffusion: Lattice-Gas Realization exhibiting Generic Two-Phase Coexistence”, *J. Chem. Phys.* 130, 074106 (2009), 15pp.
- 191.** M. Shen, D.-J. Liu, C.J. Jenks, P.A. Thiel, and J.W. Evans, “Accelerated coarsening of Ag adatom islands on Ag(111) due to trace amounts of S: Mass transport mediated by Ag-S complexes”, *J. Chem. Phys.*, 130, 094701 (2009), 13pp.
- 192.** D. Jing, B. Unal, F. Qin, J.W. Evans, C.J. Jenks, D.J. Sordelet, and P.A. Thiel, “Stranski-Krastanov-like Growth of an Ag Film on a Metallic Glass”, *Thin Solid Films*, 517, 6486-6492 (2009).
- 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”, *J. Phys. Chem. C* 113, 7277-7289 (2009).
- 194.** M. Li, C.Z. Wang, J.W. Evans, M. Hupalo, M. Tringides, and K.-M. Ho, “Competition between area and height evolution of Pb islands on a Si(111) surface”, *Phys. Rev. B* 79, 113404 (2009), 4pp.
- 195.** D.-J. Liu, H.-T. Chen, Victor S.-Y. Lin, and J.W. Evans, “Statistical mechanical modeling of catalytic polymerization within surface functionalized mesoporous materials”, *Phys. Rev. E* 80, 011801 (2009), 9pp.
- 196.** M. Albao, J.W. Evans, and F.-C. Chuang, “Kinetic Monte Carlo study on the role of defects and detachment of formation and growth of In chains on Si(100)”, *J. Phys.:Cond. Mat*, 21, 405002 (2009)
- 197.** M. Li, Y. Han, and J.W. Evans, “Comment on Capture Zone Scaling in Island Nucleation: Universal fluctuation behavior”, *Phys. Rev. Lett.* 104, 149601 (2010), 1pp.
- 198.** J.W. Evans and P.A. Thiel, “A little chemistry helps the big get bigger”, *Science* 330, 559 (2010).
- 199.** Y. Han, D.-J. Liu, B. Unal, F. Qin, D. Jing, C.J. Jenks, P.A. Thiel, and J.W. Evans, “Formation and coarsening of Ag(110) bilayer islands on NiAl(110): STM analysis and atomistic lattice-gas modeling”, *Phys. Rev. B* 81, 115462 (2010), 14pp.
- 200.** D.-J. Liu, H.-T. Chen, Victor S.-Y. Lin, and J.W. Evans, “Polymer length distributions for catalytic polymerization in mesoporous materials: Non-Markovian behavior associated with partial extrusion”, *J. Chemical Physics*, 132, 154102 (2010), 11pp.
- 201.** D.-J. Liu and J.W. Evans, “Interactions between oxygen on Pt(100): Implications for ordering during chemisorption and catalysis”, *Chem. Phys. Phys. Chem.*, 11, 2174-2181 (2010).
- 202.** M. Shen, C.J. Jenks, J.W. Evans, and P.A. Thiel, “Rapid Decay of vacancy islands at step edges on Ag(111): Step orientation dependence”, *J. Phys.: Cond. Matter*, 22, 215002 (2010), 6 pp.  
(Journal publicity at IOPscience labtalk: <http://iopscience.iop.org/0953-8984/labtalk-article/43327>)
- 203.** Y. Han, B. Unal, D. Jing, P.A. Thiel, J.W. Evans, and D.-J. Liu, “Quantum islands on metal substrates: Microscopy studies and electronic structure theory”, *Materials* 3, 3965-3993 (2010). (Special issue on Scanning Probe Microscopy – invited review).

- 204.** P. Arora, W. Li, P. Piecuch, J.W. Evans, M. Albao and M.S. Gordon, “Diffusion of atomic oxygen on the Si(100) surface”, *J. Phys. Chem. C* 114, 12649-12658 (2010).
- 205.** X. Guo, Y. de Decker, and J.W. Evans, “Metastability in a Schloegl’s second model for autocatalysis: Lattice-gas realization with particle diffusion”, *Phys. Rev. E*, 82, 021121 (2010), 12pp.
- 206.** P.A. Thiel, M. Shen, D.-J. Liu, and J.W. Evans, “Adsorbate-enhanced mass-transport on metal surfaces: oxygen and sulfur on coinage metals”, *J. Vac. Science Technol. A* 28, 1285-1298 (2010). (Invited Review + Journal Cover Image)
- 207.** G.P. Zhang, M. Hupalo, M. Li, C.Z. Wang, J.W. Evans, M.C. Tringides, and K.M. Ho, “A stochastic coarsening model for Pb islands on the Si(111) surface”, *Phys. Rev. B* 82, 165414 (2010), 5pp.
- 208.** T. Duguet, B. Unal, Y. Han, J.W. Evans, J. Ledieu, C.J. Jenks, J.M. Dubois, V. Fournee, and P.A. Thiel, “Ag thin films on the twofold surface of decagonal Al-Cu-Co quasicrystal”, *Phys. Rev. B* 82, 224204 (2010), 10 pp.

Also: 1 AIP Conference Proc. published in 2010:

---

- 209.** T. Duguet, Y. Han, C. Yuen, D. Jing, B. Unal, J.W. Evans, and P.A. Thiel, “Self-assembly of metal nanostructures on binary alloy substrates”, *Proc. Nat. Acad. Sci.*, 108, 989-994 (2011).
- 210.** D.M. Ackerman and J.W. Evans, “Boundary conditions for Burton-Cabrera-Frank type step flow models from coarse-graining of discrete 2D deposition-diffusion equations”, *SIAM Multiscale Modeling & Simulation*, 9, 59-88 (2011)
- 211.** M. Shen, C.J. Jenks, J.W. Evans, and P.A. Thiel, “How sulfur controls the nucleation of Ag islands on Ag(111)”, *Topics in Catalysis*, 54, 83-89 (2011).
- 212.** D. Ackerman, J. Wang, J.H. Wendel, D.-J. Liu, M. Pruski, and J.W. Evans, “Catalytic Conversion reactions mediated by single-file diffusion in linear nanopores: Hydrodynamic versus stochastic behavior”, *J. Chem. Phys.* 134, 114107 (2011), 13pp. (*JCP Editor’s Choice 2011*)
- 213.** A. Belianinov, B. Unal, K.-M. Ho, C.-Z. Wang, J.W. Evans, M.C. Tringides, and P.A. Thiel, “Nucleation and growth of Ag islands on the ( $\sqrt{3}\times\sqrt{3}$ )R30° phase of Ag on Si(111)”, *J. Phys. Cond. Matt.*, 23, 265002 (2011), 9pp.
- 214.** D.-J. Liu, J. Wang, D. Ackerman, I.I. Slowing, M. Pruski, H.-T. Chen, V.S.-Y. Lin, and J.W. Evans, “Interplay between anomalous transport and catalytic reaction kinetics in single-file mesoporous systems”, *ACS Catalysis* 1, 751-763 (2011) (Memorial Issue for V.S.-Y. Lin).
- 215.** Y. Han, B. Unal, D. Jing, P.A. Thiel, and J.W. Evans, “Temperature-dependent growth shapes of Ni nanoclusters on NiAl(110)”, *J. Chem. Phys.* 135, 084706 (2011), 7pp.
- 216.** C.-J. Wang, X. Guo, D.-J. Liu, and J.W. Evans, Schloegl’s second model for autocatalysis on a cubic lattice: Analysis via mean-field discrete reaction-diffusion equations, *J. Stat Phys.*, 144, 1308-1328 (2011).
- 217.** Y. Han, B. Unal, D. Jing, P.A. Thiel, and J.W. Evans, “Far-from-equilibrium growth on alloy surfaces: Ni and Al on NiAl(110)”, *Phys. Rev. B*, 84, 113414 (2011), 4pp.
- 218.** L. Roskop, J.W. Evans, and M.S. Gordon, “Adsorption and diffusion of Gallium Adatoms on the Si(100) -2x1 reconstructed surface: An MCSCF study utilizing surface clusters”, *J. Phys. Chem. C*, 115, 23488-23500 (2011).
- 219.** P.A. Thiel, B. Unal, C.Jenks, A. Goldman, P. Canfield, T. Lograsso, J.W. Evans, M. Quiquandon, D. Gratias, and M. Van Hove, “A distinctive feature of the surface structure of quasicrystals: Intrinsic and extrinsic heterogeneity” *Israel Journal of Chemistry*, 51, 1326-1339 (2011).

Also: 1 MRS Conf. Proc. article published in 2011.

---

220. Y. Han, B. Unal, and J.W. Evans, "Formation of a new type of Ni<sub>3</sub>Al surface structure by codeposition on NiAl(110)", *Physical Review Letters*, 108, 216102 (2012).
221. D.M. Ackerman, J. Wang, and J.W. Evans, "Generalized hydrodynamic treatment of the interplay between restricted transport and catalytic reactions in nanoporous materials", *Physical Review Letters*, 108, 228301 (2012).
222. A.Engstfeld, H. Hoster, R.J. Behm, L. Roelofs, X. Liu, C.-Z. Wang, Y. Han, and J.W. Evans, "Directed assembly of Ru nanoclusters on Ru(0001)-supported graphene: STM studies and atomistic modeling", *Phys. Rev. B*, 86, 085442 (2012). *PRB Editors' Suggestion*
223. X. Guo, D.K. Unruh, D.-J. Liu, and J.W. Evans, "Tricriticality in generalized Schloegl models for autocatalysis: Lattice-gas realization with particle diffusion", *Physica A* 391, 633-646 (2012).
224. Chi-Jen Wang, D.-J. Liu, and J.W. Evans, "Schloegl's second model for autocatalysis on hypercubic lattices: Dimension-dependence of generic two-phase coexistence", *Phys. Rev. E*, 85, 041109 (2012), 9pp.

Also: 3 MRS Conf. Proc. articles in 2012

---

225. S. Russell, Y. Kim, D.-J. Liu, J.W. Evans, and P.A. Thiel, "Structure, Formation, and Equilibration of Ensembles of Ag-S Complexes on an Ag Surface", *J. Chem. Phys.*, 138, 071101 (2013). (Journal of Chemical Physics Cover)
226. Y. Han, A.K. Engstfeld, R.J. Behm, and J.W. Evans, "Atomistic modeling of the directed assembly of bimetallic Pt-Ru nanoclusters on Ru(0001)-supported monolayer graphene", *J. Chem. Phys.* 138, 134703 (2013).
227. J. Wang, D.M. Ackerman, V.S.-Y. Lin, M. Pruski and J.W. Evans, "Controlling reactivity in nanoporous catalysts by tuning reaction product – pore interior interactions: statistical mechanical modeling", *J. Chem. Phys.* 138, 134705 (2013).
228. Y. Han, S.M. Russell, A.R. Layson, H. Walen, C. D. Yuen, P.A. Thiel, and J.W. Evans, "Anisotropic coarsening: One-dimensional decay of Ag islands on Ag(110)", *Phys. Rev. B* 87, 155420 (2013).
229. C.-J. Wang, Y. Han, H. Walen, S.M. Russell, P.A. Thiel, and J.W. Evans, "Analytic formulations for one-dimensional decay of rectangular homoepitaxial islands during coarsening on anisotropic fcc(110) surfaces", *Phys. Rev. B*, 88, 155434 (2013).

Also Major 128 p. Report in high-impact Review Journal in 2013:

D.-J. Liu and J.W. Evans, "Realistic multisite lattice-gas modeling and KMC simulation of catalytic surface reactions: Kinetics and multiscale spatial behavior for CO-oxidation on metal(100) surfaces", *Progress in Surface Science*, 88, 393-521 (2013). (128 pages)

Also: 2 MRS Conf. Proc. articles for 2013.

J.W. Evans, P.A. Thiel, and B. Unal, "Atomistic and coarse-grained modeling strategies for thin film nucleation and growth on quasicrystalline surfaces", *MRS Symp. Proc. Vol. 1517* (MRS, Pittsburgh, 2013)  
DOI: 10.1557/opl.2012.1753

Y. Han, A.K. Engstfeld, C.Z. Wang, L.D. Roelofs, R.J. Behm, and J.W. Evans, "Atomistic modeling of Ru NC formation on graphene/Ru(0001): Thermodynamic vs. kinetic directed-assembly", *MRS Symp. Proc. Vol. 1498* (MRS, Pittsburgh, 2013) DOI: 10.1557/opl.2013.106

---

- 230.** C.-J. Wang, D.M. Ackerman, I.I. Slowing, and J.W. Evans, “Langevin and Fokker-Planck analyses of inhibited molecular passing processes controlling transport and reactivity in nanoporous materials”, *Phys. Rev. Lett.* 113, 038301 (2014).
- 231.** Y. Han, D.-J. Liu, and J.W. Evans, Real-time ab-initio KMC simulation of the self-assembly and sintering of bimetallic nanoclusters on fcc(100) surfaces: Au+Ag on Ag(100), *Nano Letters*, 14, 4646-4652 (2014).
- 232.** B. Ünal, J.W. Evans, and P.A. Thiel, Temperature dependence of Ag film roughening during deposition on quasicrystal and approximant surfaces, *Acta Phys. Polonica A*, 126, 608-612 (2014). (*Proceedings of the 12<sup>th</sup> International Conference on Quasicrystals*)
- 233.** D.-J. Liu and J.W. Evans, “Dissociative adsorption of O<sub>2</sub> on unreconstructed metal(100) surfaces: Pathways, energetics, and sticking kinetics”, *Phys. Rev. B* 89, 205406 (2014)
- 234.** J.W. Evans and D.-J. Liu, “Statistical mechanical models for dissociative adsorption of O<sub>2</sub> on metal(100) surfaces with blocking, steering, and funneling”, *J. Chem. Phys.* 140, 194704 (2014).
- 235.** D. Appy, H. Lei, C.-Z. Wang, M.C. Tringides, D.-J. Liu, J.W. Evans, and P.A. Thiel, “Transition and Noble Metals on the (0001) Surface of Graphite: Fundamental Aspects of Adsorption, Diffusion, and Morphology”, *Progress in Surface Science*, 89, 219-238 (2014).
- 236.** D.-J. Liu, H. Walen, J. Oh, H. Lim, J.W. Evans, Y. Kim, P.A. Thiel, “A search for the structure of sulfur-induced reconstruction on Cu(111), *J. Phys. Chem. C*, 118, 29218-29223 (2014).
- 237.** D. Appy, H. Lei, Y. Han, C.-Z. Wang, M.C. Tringides, E.J. Kwolek, J. W. Evans, and P. A. Thiel, Copper nanoclusters on the basal plane of graphite: Experimental and theoretical elucidation of the formation mechanism, *Phys. Rev. B*, 90, 195406 (2014).

Also: 1 MRS Conf. Proc. article for 2014.

Jing Wang, Andrés Garcia, David M. Ackerman, Mark S. Gordon, Igor I. Slowing, Takeshi Kobayashi, Marek Prusk and James W. Evans, Multi-functionalization of nanoporous catalytic materials to enhance reaction yield: Statistical mechanical modeling for conversion reactions with restricted diffusive transport, *Mater. Res. Soc. Symp. Proc. Vol. 1641 @ 2014 Materials Research Society DOI: 10.1557/opl.2014.321.*

- 238.** Y. Han and J.W. Evans, “Directing anisotropic assembly of metallic nanoclusters by exploiting linear trio interactions and quantum size effects: Au chains on Ag(100) thin films”, *J. Physical Chemistry Letters*, 6, 2194-2199 (2015).
- 239.** H. Walen, D.-J. Liu, J. Oh, H. Lim, J. W. Evans, C. Aikens, Y. Kim, and P. A. Thiel, Cu<sub>2</sub>S<sub>3</sub> complex on Cu(111) as a candidate for mass transport enhancement, *Phys. Rev. B*, 91, 045426 (2015), 6pp.
- 240.** D.-J. Liu and J.W. Evans, “Transitions between strongly correlated and random steady-states for catalytic CO-oxidation on surfaces at high-pressure”, *J. Chem. Phys.* 142, 134703 (2015), 15pp.
- 241.** C.-J. Wang, D.-J. Liu, and J.W. Evans, “Discontinuous non-equilibrium phase transition in a threshold version of Schloegl’s model for autocatalysis: Generic two-phase coexistence and metastability”, *J. Chem. Phys.* 142, 164105 (2015), 12pp.
- 242.** H. Walen, D.-J. Liu, J. Oh, H. Lim, J. W. Evans, Y. Kim, and P. A. Thiel  
Reconstruction of Steps on the Cu(111) Surface Induced by Sulfur, *J. Chem. Phys.* 142, 194711 (2015), 15pp
- 243.** R. Zhao, D.M. Ackerman, and J.W. Evans, Refined BCF-type boundary conditions for mesoscale surface step dynamics, *Phys. Rev. B*, 91, 235441 (2015), 10pp.
- 244.** H. Walen, D.-J. Liu, J. Oh, H. Lim, J. W. Evans, Y. Kim, and P. A. Thiel  
Self-Organization of S Adatoms on Au(111):  $\sqrt{3}R30^\circ$  Rows at Low Coverage, *J. Chem. Phys.* 143, 014704 (2015), 10pp.

**245.** Y. Han and J.W. Evans, Adsorption and diffusion of Ru adatoms on Ru(0001)-supported graphene: large-scale first-principles calculations, *J. Chem. Phys.* 143, 164706 (2015).

Also major Reviews in *Chem. Rev.* 72 pp. (IF = 45) and *Prog. Surf. Sci.* 47 pp. (IF = 9.0 ) for 2015:

D.-J. Liu, A. Garcia, J. Wang, D.M. Ackerman, C.-J. Wang, and J.W. Evans, “Kinetic Monte Carlo simulation of statistical mechanical models and coarse-grained mesoscale descriptions of catalytic reaction-diffusion processes: 1D nanoporous and 2D surface systems”, *Chemical Reviews*, 115, 5979-6050 (2015), 72 pp.

X. Liu, Y. Han, J.W. Evans, A. Engstfeld, R.J. Behm, M.C. Tringides, M. Hupalo, H.-Q. Lin, L. Huang, K.-M. Ho, D. Appy, P.A. Thiel, and C.Z. Wang, Growth morphology and properties of metals on graphene, *Progress in Surf. Sci.*, 90, 397-443 (2015), 47 pp.

---

**246.** W.-K. Huang, K.-W. Zhang, C.-L. Yang, H. Ding, X. Wan, S.-C. Li, J.W. Evans, and Y. Han, Tailoring kinetics on a topological insulator surface by defect-induced strain: Pb mobility on Bi<sub>2</sub>Te<sub>3</sub>, *Nano Letters*, 16, 4454-4461 (2016).

**247.** W. Li, L. Huang, J.W. Evans, and Y. Han, Submonolayer Ag films on Fe(100): First-principles analysis of energetics controlling adlayer thermodynamics and kinetics, *Phys. Rev. B*, 93, 155416 (2016), 13 pp.

**248.** R. Zhao, J.W. Evans,\* and T.J. Oliveira, Permeability and kinetic coefficients for mesoscale BCF surface step dynamics: Discrete 2D deposition-diffusion equation analysis, *Phys. Rev. B*, 93, 165411 (2016), 15 pp. \*Corresponding Author.

249. E. Kwolek, H. Lei, A. Lii-Rosales, M. Wallingford, Y. Zhou, C.-Z. Wang, M.C. Tringides, J.W. Evans, and P.A. Thiel, Adsorption of Dy on the Graphite (0001) Surface: Nucleation & Growth at 300 K, *J. Chem. Phys.* 145, 211902 (2016), 8 pp. Special Topic Issue on Nucleation.

**250.** J. Boschen, J. Lee, T.L. Windus, J.W. Evans, and D.-J. Liu, Size-dependence of S-bonding on (111) facets of Cu nanoclusters, *J. Phys. Chem. C*, 120, 10268-10274 (2016).

**251.** A. Garcia, J. Wang, T.L. Windus, A.D. Sadow, and J.W. Evans, Catalytic conversion reactions in nanoporous systems with concentration-dependent selectivity: Statistical mechanical modeling, *Phys. Rev. E*, 93, 052137 (2016), 12 pp.

**252.** Y. Han, E. Gaudry, T.J. Oliveira, and J.W. Evans, Point island models for nucleation and growth of supported nanoclusters during surface deposition, *J. Chem. Physics*, 145, 211904 (2016), 14pp. Special Topic Issue on Nucleation.

**253.** Y. Han, M. Li, and J.W. Evans, Scaling of capture zone area distributions for nucleation and growth of islands during submonolayer deposition, *J. Chem. Physics*, 145, 211911 (2016), 12 pp. Special Topic Issue on Nucleation

<https://publishing.aip.org/publishing/journal-highlights/location-matters-self-assembly-nanoclusters>

**254.** Y. Han, C.R. Stoldt, P.A. Thiel, and J.W. Evans, Ab Initio Thermodynamics and Kinetics for Coalescence of Two-Dimensional Nanoislands and Nanopits on Metal (100) Surfaces, *J. Phys. Chem. C*, 120, 21617-21630 (2016).

**255.** J. Boschen, J. Lee, T.L. Windus, J.W. Evans, P.A. Thiel, and D.-J. Liu, Comparison of S-adsorption on (111) and (100) facets of Cu nanoclusters, *J. Chem. Phys.*, 145, 164312 (2016), 8 pp.

**256.** A. Garcia and J. W. Evans, Catalytic Conversion in Nanoporous Materials: Concentration Oscillations and Spatial Correlations due to Inhibited Transport and Intermolecular Interactions, *J. Chem. Phys.*, 145, 174705 (2016), 11 pp.

**257.** D.-J. Liu, F. Zahariev, M.S. Gordon, and J.W. Evans, Predictive Beyond-Mean-Field Rate Equations for Multisite Lattice-Gas Models of Catalytic Surface Reactions: CO-Oxidation on Pd(100) , *J. Phys. Chem. C*, 120, 28639-28653 (2016).

---

- 258.** D.M. Ackerman and J.W. Evans, Tracer counter-permeation analysis of diffusivity in finite-length nanopores with and without single-file dynamics, *Phys. Rev. E*, 95, 012132 (2017), 12 pp.
- 259.** A. García and J.W. Evans, Boundary conditions for diffusion-mediated processes within linear nanopores: Exact treatment of coupling to an equilibrated external fluid, *J. Phys. Chem. C*, 121, 8873-8888 (2017).
- 260.** Y. Han, A. Lii-Rosales, Y. Zhou, C.-J. Wang, M. Kim, M.C. Tringides, C.-Z. Wang, P.A. Thiel, and J.W. Evans, Nucleation and growth kinetics for intercalated islands during deposition on layered materials with isolated point-like surface defects, *Phys. Rev. Materials*, 1, 053403 (2017), 10pp.
261. W. Li, H. Wei, P. Li, G.S. Raj, G.-H. Lu, F. Liu, J.W. Evans, and Y. Han, Thickness-dependent energetics for Pb adatoms on low-index Pb nano film surfaces: 1<sup>st</sup>-principles calculations, *Phys. Rev. B*, 96, 205409 (2017), 14pp.
- 262.** K.C. Lai, J.W. Evans,\* and D.-J. Liu, Communication: Diverse nanoscale cluster dynamics: Diffusion of 2D epitaxial clusters, *J. Chem. Phys.*, 147, 201101 (2017), 4pp. \*Corresponding Author.
263. K.C. Lai, D.-J. Liu, and J.W. Evans, Diffusion of 2D epitaxial clusters on metal(100) surfaces: Facile versus nucleation-mediated behavior and their merging for larger sizes, *Phys. Rev. B*, 96, 235406 (2017), 15 pp.
- 
- 264.** D.-J. Liu, C.-J. Wang, and J.W. Evans, Discontinuous phase transitions in non-local Schloegl models for autocatalysis: Loss and reemergence of a non-equilibrium Gibbs phase rule, *Physical Review Letters*, 121, 120603 (2018), 6 pp.
- 265.** D.-J. Liu, J. Lee, T.W. Windus, P.A. Thiel, and J.W. Evans, Stability of M<sub>3</sub>S<sub>3</sub> complexes on fcc M(111) surfaces: M = Au, Ag, Cu, and Ni, *Surface Science*, 676, 2-8 (2018) P.R. Norton Special Issue.
- 266.** K.C. Lai, D.-J. Liu, P.A. Thiel, and J.W. Evans, Modeling of diffusivity for 2D vacancy pits and comparison with 2D adatom islands on metal(100) surfaces including analysis for Ag(100), *J. Phys. Chem. C*, 122, 11334-11344 (2018). *J. Phys. Chem. C Journal Cover*
- 267.** A. Lii-Rosales, Y. Han, J.W. Evans, D. Jing, Y. Zhou, M.C. Tringides, M. Kim, C.-Z. Wang, P.A. Thiel, Formation of Multilayer Cu Islands Embedded beneath the Surface of Graphite: Characterization and Fundamental Insights, *J. Phys. Chem. C*, 122, 4454-4469 (2018). *J. Phys. Chem. C Journal Cover*
268. A. Lii-Rosales, Y. Han, K.M. Yu, D. Jing, N. Anderson, D. Vaknin, M. Tringides, J.W. Evans, M. Altman, and P.A. Thiel, Reverse-Engineering of Graphene on Metal Surfaces: A Case Study of Embedded Ruthenium, *Nanotechnology*, 29, 505601 (2018), 14 pp.
- 269.** A. Garcia, I.I. Slowing, and J.W. Evans, Pore diameter dependence of catalytic activity: PNB conversion to an aldol product in amine-functionalized mesoporous silica, *J. Chem. Phys.* 149, 024101 (2018), 12pp.
- 
- 270.** K.C. Lai and J.W. Evans, Reshaping and sintering of 3D fcc metal nanoclusters: Stochastic atomistic modeling with realistic surface diffusion kinetics, *Phys. Rev. Materials* 3, 026001 (2019), 10pp.
- 271.** M. Chen, Y. Han, T.W. Goh, R. Sun, R.V. Maligal-Ganesh, Y. Pei, C.-K. Tsung, J.W. Evans\*, and W. Huang\*, Kinetics, Energetics, and Size-dependence of the Transformation from Pt to Ordered PtSn Intermetallic Nanoparticles, *Nanoscale*, 11, 5336-5345 (2019) \*Corresponding Authors.
- 272.** S.E. Julien, A. Lii-Rosales, K.-T. Wan, Y. Han, M.C. Tringides, J.W. Evans, and P.A. Thiel, Squeezed Nanocrystals: Equilibrium Configuration of Metal Clusters Embedded Beneath the Surface of a Layered Material, *Nanoscale*, 11, 6445-6452 (2019) One of *Most Popular Articles 2019*
- 273.** Y. Han, K.C. Lai, A. Lii-Rosales, M.C. Tringides, J.W. Evans, and P.A. Thiel, Surface energies, adhesion energies, and exfoliation energies relevant to Cu-graphene & Cu-graphite systems, *Surface Science*, 685, 48-58 (2019). *Surface Science partial Journal Cover.*

**274.** Y. Han, A. Lii-Rosales, M.C. Tringides, J.W. Evans, P.A. Thiel, Energetics of Cu adsorption and intercalation at graphite step edges, *Phys. Rev. B*, 99, 115415 (2019), 11pp.

**275.** K.C. Lai, X. Zha, J.W. Evans, and A. Travesset, Structure of Polydisperse fcc Nanocrystals: Implications for Crystal Fractionalization, *J. Phys. Chem. C*, 123, 9528-9537 (2019).

**276.** J. Lee, T.L. Windus, P.A. Thiel, J.W. Evans, and D.-J. Liu, Coinage Metal-Sulfur Complexes: Stability on Metal(111) Surfaces and in the Gas Phase, *J. Phys. Chem. C*, 123, 12954-12965 (2019).

**277.** K.C. Lai and J.W. Evans, Complex oscillatory decrease with size in diffusivity of (100)-epitaxially supported 3D fcc nanoclusters, *Nanoscale*, 11, 17506-17516 (2019).

**278.** A. Lii-Rosales, Y. Han, K.C. Lai, D. Jing, M.C. Tringides, J.W. Evans, and P.A. Thiel, Fabricating metallic Fe nanocrystals via encapsulation at the graphite surface, *J. Vac. Science & Technology A*, 37, 061403 (2019), 15 pp.  
*JVSTA Featured Article*

**279.** Y. Han, J.W. Evans, and F. Liu, Energy barriers for Pb adatom diffusion on stepped ultrathin Pb(111) quantum nanofilms: first-principles calculations, *Phys. Rev. B*, 100, 195405 (2019), 8pp.

**280.** D.-J. Liu, P.M. Spurgeon, J. Lee, T.L. Windus, P.A. Thiel, and J.W. Evans, Sulfur adsorption on coinage metal (100) surfaces: Propensity for metal-sulfur complex formation relative to (111) surfaces, *Physical Chemistry Chemical Physics* 21, 26483-26491 (2019).

Also in 2019: Major Review: King C. Lai, Yong Han, Peter Spurgeon, Wenyu Huang, Patricia A. Thiel, Da-Jiang Liu, and James W. Evans, Reshaping, intermixing, and coarsening of metallic nanocrystals: Non-equilibrium statistical mechanical & coarse-grained modeling, *Chem. Rev.* 119, 6670-6768 (2019).

*Chemical Reviews supplementary Journal Cover*

**281.** K. C. Lai, M. Chen, B. M. Williams, Y. Han, C.-K. Tsung, W. Huang, and J. W. Evans, Reshaping of Truncated Pd Nanocubes: Energetic and Kinetic Analysis Integrating Transmission Electron Microscopy with Atomistic-Level and Coarse-Grained Modeling, *ACS Nano*, 14, 8551-8561 (2020).

**282.** Lin Wei, Da-Jiang Liu, Bryan A. Rosales, James W. Evans, and Javier Vela, Selective Hydrogenation of Aqueous Nitrate to Ammonia over Ni<sub>2</sub>P, *ACS Catalysis*, 10, 3618-3628 (2020).

**283.** B. Williams, A. Young, I. Andoni, Y. Han, W.-S. Lo, J. Yang, M. Golden, C.-R. Kao, C.-H. Kuo, J.W. Evans, W. Huang, and C.-K. Tsung, Strain-Driven Metallic Intermixing in Shape-Controlled Multi-layered Core-Shell Nanostructures: Toward Shaped Intermetallics, *Angew. Chem. (Int. Ed.)* 59, 2-9 (2020).

**284.** W. Li, L. Huang, M.C. Tringides, J.W. Evans, and Y. Han, Thermodynamic Preference for Atom Adsorption on versus Intercalation into Multilayer Graphene, *J. Phys. Chem. Lett.* 11, 9725-9730 (2020).

**285.** Linxia Wang, King C. Lai, Li Huang, James W. Evans, and Yong Han, Low-index surface energies, cleavage energies, and surface relaxations for crystalline NiAl from first-principles calculations, *Surface Science*, 695, 121532 (2020), 11pp.  
*Surface Science Journal Cover*

**286.** Chi-Jen Wang, Da-Jiang Liu, and James W. Evans, Extended families of critical and stationary droplets for non-equilibrium phase transitions in spatially-discrete bistable systems, *Phys. Rev. E*, 101, 022803 (2020), 9 pp.

**287.** A. Lii-Rosales, Y. Han, S. Julien, O. Pierre-Louis, D. Jing, W.-T. Wan, M.C. Tringides, J.W. Evans, P.A. Thiel, Shapes of Fe nanocrystals encapsulated at the graphite surface, *New J. Physics*, 22, 023106 (2020), 16pp.

**288.** D. Jing, A. Lii-Rosales, K.C. Lai, Q. Li, J. Kim, M.C. Tringides, J.W. Evans, and P.A. Thiel, Far-From-Equilibrium Growth of Metal Clusters on a Layered Material: Cu on MoS<sub>2</sub>, *New J. Phys.* 22, 053033 (2020), 11 pp.

**289.** Yong Han, Michael C. Tringides, James W. Evans, and Patricia A. Thiel, Adsorption, intercalation, diffusion, and adhesion of Cu at the 2H-MoS<sub>2</sub>(0001) surface from first-principles calculations



Phys. Rev. Research 2, 013182 (2020), 11 pp.

**290.** P.M. Spurgeon, K.C. Lai, Y. Han, J.W. Evans,\* and P.A. Thiel,\* Fundamentals of Au(111) Surface Dynamics: Coarsening of 2D Au Islands, *J. Phys. Chem. C*, 124, 7492-7499 (2020).

*J. Phys. Chem. C supplementary Journal Cover*

**291.** J. Sebastián Manzano, H. Wang, T. Kobayashi, P. Naik, K.C. Lai, J.W. Evans, and I.I. Slowing, Kinetics of the Functionalization of Mesoporous Silica Nanoparticles with Organotrialkoxysilanes, *Microporous & Mesoporous Materials*, 305, 110276 (2020), 9 pp.

**292.** King C. Lai, Tyler J. Pleasant, Andres Garcia, and James W. Evans, Generalized hydrodynamic analysis of transport through finite open nanopores in two-component single-file systems, *Phys. Rev. E*, 101, 062103 (2020), 10 pp.

**293.** Da-Jiang Liu, James W. Evans\*, Peter M. Spurgeon, and Patricia A. Thiel\*, Structure of Chalcogen Overlayers on Au(111): Density Functional Theory and Lattice-Gas Modeling, *J. Chem. Phys.*, 152, 224706 (2020), 10 pp.

**294.** K.C. Lai, A. Lii-Rosales, and J.W. Evans, Equilibrium Shapes of Faceted 3D Metal Nanoclusters Intercalated near the Surface of Layered Materials, *J. Phys.: Cond. Matter*, 32, 445001 (2020), 9 pp.

**295.** Y. Han, I.I. Slowing, and J.W. Evans, Surface structure of linear nanopores in amorphous silica: Comparison of pore generation algorithms, *J. Chem. Phys.*, 153, 124708 (2020), 11pp.

Also in 2020: 1 book chapter: A. Garcia, C.-J. Wang, D.M. Ackerman, M.S. Gordon, I.I. Slowing and J.W. Evans, Anomalous Kinetics of Catalytic Conversion Reactions in Linear Nanopores mediated by Inhibited Transport: Multiscale Modeling, Chapter 7 in "Chemical Kinetics beyond the Textbook" (World Scientific, Singapore, 2020), pp. 173-190. Ed. K. Lindenberg, R. Metzler, G. Oshanin. [https://doi.org/10.1142/9781786347015\\_0007](https://doi.org/10.1142/9781786347015_0007)

**296.** King C. Lai, Minda Chen, Jiaqi Yu, Yong Han, Wenyu Huang, and James W. Evans,\* Shape stability of truncated octahedral fcc metal nanocrystals, *ACS Applied Mat. Interfaces*, 13, 51954-51961 (2021). <https://doi.org/10.1021/acsami.1c07894>

**297.** Ann Lii-Rosales,\* Yong Han, Dapeng Jing, Michael C. Tringides, Scott Julien, Kai-Tak Wan, Cai-Zhuang Wang, King C. Lai, J.W. Evans,\* and Patricia A. Thiel, Encapsulation of Metal Nanoparticles at the Surface of a Prototypical Layered Material, *Nanoscale*, 13, 1485-1506 (2021)  
DOI: 10.1039/D0NR07024F

**298.** Chen Liu, Yinong Zhou, Guanyong Wang, Yin Yin, Haili Huang, Jiayi Chen, Jiaying Liu, Dandan Guan, Yaoyi Li, Shiyong Wang, Hao Zheng, Canhua Liu, Yong Han,\* James W. Evans, Feng Liu, and Jinfeng Jia,\* Sierpiński Structure and Electronic Topology in Bi Thin Films on InSb(111)B Surfaces, *Physical Review Letters*, 126, 176102 (2021). DOI: 10.1103/PhysRevLett.126.176102

**299.** Yong Han, A. Lii-Rosales, M.C. Tringides, and James W. Evans\*, Competitive formation of intercalated versus supported metal nanoclusters during deposition on layered materials with surface point defects, *J. Chem. Phys.* 154, 024703 (2021), 8pp. DOI: 10.1063/5.0037480

**300.** Peter M. Spurgeon, Da-Jiang Liu, T. L. Windus, James W. Evans,\* and Patricia A. Thiel, Enhanced dynamics of nanostructures on Au(111) with adsorbed S due to Au-S complex formation, *ChemPhysChem*, 22, 349-358 (2021). [doi.org/10.1002/cphc.202000884](https://doi.org/10.1002/cphc.202000884) *Journal Cover*

*Also:* P.M. Spurgeon, D.-J. Liu, T.L. Windus, J.W. Evans,\* and P.A. Thiel, **Cover Profile:** Enhanced dynamics of nanostructures on Au(111).. *ChemPhysChem*, 22 (2021). [doi.org/10.1002/cphc.202100060](https://doi.org/10.1002/cphc.202100060)

**301.** Yue Liu, Xiaojie Liu, Cai-Zhuang Wang,\* Yong Han, James W. Evans, Ann Lii-Rosales, Michael C. Tringides and Patricia A. Thiel, Mechanism of metal intercalation under graphene through small vacancy defects, *J. Phys. Chem. C*, 125, 6954-6962 (2021). DOI: 10.1021/acs.jpcc.1c00814

**302.** Yu Lim Kim, Yong Han, James W. Evans\* and Mark S. Gordon\*, Effective Fragment Potential based Molecular Dynamics Studies of Diffusion in Acetone and Hexane, *J. Phys. Chem. A*, 125, 3398-3405 (2021). DOI: 10.1021/acs.jpca.1c01865

- 303.** Da-Jiang Liu, Chi-Jen Wang, and James W. Evans,\* Phase transitions in Schloegl's second model for autocatalysis on a Bethe lattice, *Phys. Rev. E*, 104, 014135 (2021).  
<https://doi.org/10.1103/PhysRevE.104.014135>
- 304.** Yong Han\*, James W. Evans, and Michael C. Tringides, Dy adsorption on and intercalation under graphene on 6H-SiC(0001) surface from first-principles calculations, *Phys. Rev. Materials*, 5, 074004 (2021) <https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.5.074004>
- 305.** Yong Han\*, James W. Evans, and Michael C. Tringides, Energy barriers for Dy and H penetration through unsupported graphene and graphene unsupported on 6H-SiC(0001) from first-principles calculations, *Applied Phys. Lett.*, 119, 033101 (2021) <https://doi.org/10.1063/5.0056916>
- 306.** Yong Han, Dapeng Jing, Yilong Luan, Chi-Jen Wang, Marek Kolmer, Zhe Fei, Michael C. Tringides, and James W. Evans, Thermodynamically-driven Formation of Intercalated Cu Carpets from Supported Cu Pyramids on MoS<sub>2</sub>, *J. Phys. Chem. Lett.*, 13, 6651-6656 (2022).  
<https://doi.org/10.1021/acs.jpcclett.2c01458> *Supplementary Journal Cover*
- 307.** D.-J. Liu and J.W. Evans, Sulfur-enhanced dynamics of coinage metal(111) surfaces: Step edges vs terraces as locations for metal-sulfur complex formation, *J. Vac. Sci. Technol. A* 40, 023205 (2022)  
<https://doi.org/10.1116/6.0001408> Selected as *Featured Article*, partial *Journal Cover*
- 308.** Yu Lim Kim, Mark S. Gordon, Andres Garcia, and James W. Evans, Rotational and translational diffusion of liquid n-hexane: EFP-based Molecular Dynamics analysis, *J. Chem. Phys.* 156, 114503 (2022). <https://doi.org/10.1063/5.0079212>
- 309.** Ellie L. Fought, Yong Han, Theresa L. Windus, Igor I. Slowing, Takeshi Kobayashi, James W. Evans, Modeling of linear nanopores in a-SiO<sub>2</sub> tuning pore surface structure, *Microporous & Mesoporous Materials* 341, 112077 (2022), 9 pp. <https://doi.org/10.1016/j.micromeso.2022.112077>
- 310.** D.-J. Liu and J.W. Evans, Reaction processes at step edges on S-decorated Cu(111) and Ag(111) surfaces: MD analysis utilizing Machine Learning derived potentials, *J. Chem. Phys.* **156**, 204106 (2022); <https://doi.org/10.1063/5.00892100>
- 311.** Y. Han,\* J.W. Evans, and M.C. Tringides, Thermodynamics and kinetics of H adsorption and intercalation for graphene on 6H-SiC(0001) from first-principles calculations, *J. Vac. Sci. Technol. A*, 40, 012202 (2022). <https://doi.org/10.1116/6.0001343>
- 312.** Yu Lim Kim, J.W. Evans, and M.S. Gordon, Molecular interactions in diffusion-controlled aldol condensation with mesoporous silica nanoparticles, *Phys. Chem. Chem. Phys.* 24, 10475-10497 (2022).  
<https://doi.org/10.1039/D2CP00952H>
- 313.** D. Jing, Y. Han, J.W. Evans, M. Kolmer, Z. Fei, and M.C. Tringides, Unusual flat and extended morphology of encapsulated Cu under MoS<sub>2</sub>, *Phys. Rev. Materials*, 6, 094008 (2022), 10 pp.  
<https://doi.org/10.1103/PhysRevMaterials.6.094008>
- Also:* D.A. Chen, A. Lii-Rosales, and J.W. Evans,\* Preface: Special Collection commemorating the career of Pat Thiel, *J. Vac. Sci. Technol. A*, 40, 031601 (2022), 2 pp. <https://doi.org/10.1116/6.0001807>
- 314.** King C. Lai, Da-Jiang Liu and James W. Evans, Nucleation-mediated reshaping of faceted metallic nanocrystals: Breakdown of the classical free energy picture, *J. Chem. Phys.* 158, 104102 (2023), 10 pp.  
*Editor's Pick* <https://doi.org/10.1063/5.0138266>
- 315.** King C. Lai, Charles T. Campbell, and James W. Evans, Size-dependent diffusion of supported metal nanoclusters: Mean-field-type treatments and beyond for faceted clusters, *Nanoscale Horizons*, 8, 1556-1567 (2023). <https://doi.org/10.1039/D3NH00140G> *Inside Cover*
- 316.** Y. Han, M. Kolmer, M.C. Tringides, and J.W. Evans, Thermodynamics and Kinetics of Pb Intercalation under Graphene on SiC(0001), *Carbon*, 205, 336-344 (2023).  
<https://doi.org/10.1016/j.carbon.2023.01.029>

- 317.** Yong Han, Puranjan Chatterjee, Sardar B. Alam, Tanya Prozorov, Igor I. Slowing and James W. Evans, Interlayer spacing in pillared and grafted MCM-22 type silicas: Density functional theory analysis versus experiment, *PhysChemChemPhys*, 25, 4680-4689 (2023). <https://doi.org/10.1039/d2cp03391g>
- 318.** Zheren Shen, Da-Jiang Liu, and James W. Evans, Generic two-phase coexistence in a type-2 Schloegl model for autocatalysis on a square lattice: Analysis via heterogeneous master equations, *Phys. Rev. E*, 107, 034104 (2023), 8 pp. <https://doi.org/10.1103/PhysRevE.107.034104>
- 319.** Da-Jiang Liu and James W. Evans, Fluorine spillover for ceria- vs silica-supported palladium nanoparticles: a MD study using machine learning potentials, *J. Chem. Phys.* 159, 024101 (2023). <https://doi.org/10.1063/5.0147132>
- 320.** Pranjali Naik, Pranaw Kunal, Da-Jiang Liu, James W. Evans, Igor I. Slowing, Efficient Transfer Hydrodehalogenation of Halophenols Catalyzed by Pd Supported on Ceria, *Applied Catal. A* 650, 119007 (2023), 9 pp. <https://doi.org/10.1016/j.apcata.2022.119007>
- 321.** Y. Han,\*, S. Chen, J. Hall, S. Roberts, M. Kolmer, J.W. Evans, and M.C. Tringides, Degeneracy in Intercalated Pb Phases under Buffer-Layer Graphene on SiC(0001) and Diffuse Moiré Spots in Surface Diffraction, *J. Phys. Chem. Letters*, 14, 7053-7058 (2023). <https://doi.org/10.1021/acs.jpcclett.3c01688>
- 322.** S. Chen, J. Hall, M. Kolmer, M. Hupalo, Y. Han, J.W. Evans, and M.C. Tringides, Targeted Dy intercalation under Gr/SiC for tuning its electronic band structure, *Phys. Rev. B* 107, 045408 (2023), 12 pp. <https://doi.org/10.1103/PhysRevB.107.045408>
- 323.** P. Chatterjee, Y. Han, T. Kobayashi, K.K. Verma, R.K. Behera, T.H. Johnson, T. Prozorov, J.W. Evans, I.I. Slowing, and W. Huang, Capturing rare earth elements by synthetic aluminosilicate MCM-22: Mechanistic understanding of Yb<sup>3+</sup> capture, *ACS Applied Materials & Interfaces* 15, 54192-54201 (2023). <https://doi.org/10.1021/acsami.3c14560>
- 324.** Yong Han and James W. Evans, Real-time KMC simulation of vacancy-mediated intermixing in Au@Ag octahedral core – cubic shell nanocrystals with *ab-initio*-guided kinetics, *ACS Nano*, in press (2024). <https://doi.org/10.1021/acsnano.4c06435>
- 325.** King C. Lai, Da-Jiang Liu, Wenyu Huang, Yong Han, and James W. Evans, Thermal shape stability of fcc metal nanocrystals synthesized with faceted non-equilibrium shapes, *J. Phys. Chem. C*, 128, 7026-7040 (2024) *Invited Review, Suppl. Cover* <https://doi.org/10.1021/acs.jpcc.4c00752>
- 326.** Yong Han, Tamalika Ash, Puranjan Chatterjee, Wenyu Huang, Theresa L. Windus, and James W. Evans, DFT analysis of the binding of rare earth nitrates at internal and external surfaces of MCM-22, *J. Phys. Chem. C*, 128, 6309-6318 (2024) *Suppl. Cover* <https://doi.org/10.1021/acs.jpcc.4c00117>
- 327.** Dapeng Jing, Yong Han, Marek Kolmer, Michael C. Tringides, James W. Evans, Crystal structure and shape selection in the growth of 3D metallic clusters on layered materials: Fe on MoS<sub>2</sub>, *Surface Science*, 747, 122522 (2024), 9 pp. *Front Cover* <https://doi.org/10.1016/j.susc.2024.122522>
- 328.** Yong Han and James W. Evans, Versatile stochastic model for predictive KMC simulation of fcc metal nanostructure evolution with realistic kinetics, *J. Chem. Phys.*, 161 074108 (2024), 11 pp. <https://doi.org/10.1063/5.0221012>
- 329.** Yong Han,\* Marek Kolmer, James W. Evans, and Michael C. Tringides, First-principles analysis of intercalated Pb structures under buffer-layer graphene on SiC(0001): Pb(111)-, plumbene-, and amorphous-like Pb layers, *Phys. Rev. Materials*, 8, 044002 (2024), 16 pp. <https://doi.org/10.1103/PhysRevMaterials.8.044002>
- 330.** Yong Han, Da-Jiang Liu, K.C. Lai, P.A. Thiel, and James W. Evans, Formation and coarsening of epitaxially-supported metal nanoclusters, *Surface Science* (2024) (invited for “60 Years” special issue)

\*Corresponding author(s) when not the last author.

**MAJOR REVIEWS**

- R1. J. W. Evans, “Random and Cooperative Sequential Adsorption”, *Reviews of Modern Physics*, 65, 1281-1329 (1993). 48 pp.
- R2. J. W. Evans, P. A. Thiel and M. C. Bartelt, “Morphological Evolution during Epitaxial Thin Film Growth: Formation of 2D Islands and 3D Mounds,” *Surface Science Reports*, 61, 1-128 (2006). 128 pp.
- R3. D.-J. Liu and J.W. Evans, “Realistic multisite lattice-gas modeling and KMC simulation of catalytic surface reactions: Kinetics and multiscale spatial behavior for CO-oxidation on metal(100) surfaces”, *Progress in Surface Science*, 88, 393-521 (2013). 128 pp.
- R4. X. Liu, Y. Han, J.W. Evans, A. Engstfeld, R.J. Behm, M.C. Tringides, M. Hupalo, H.-Q. Lin, L. Huang, K.-M. Ho, D. Appy, P.A. Thiel, and C.Z. Wang, Growth morphology and properties of metals on graphene, *Progress in Surface Science*, 90, 397-443 (2015). 47 pp.
- R5. D.-J. Liu, A. Garcia, J. Wang, D.M. Ackerman, C.-J. Wang, and J.W. Evans, “Kinetic Monte Carlo simulation of statistical mechanical models and coarse-grained mesoscale descriptions of catalytic reaction-diffusion processes: 1D nanoporous and 2D surface systems”, *Chemical Reviews*, 115, 5979-6050 (2015). 71 pp.
- R6. K.C. Lai, Y. Han, P. Spurgeon, W. Huang, P.A. Thiel, D.-J. Liu, and J.W. Evans, Reshaping, intermixing, and coarsening of metallic nanocrystals: Non-equilibrium statistical mechanical and coarse-grained modeling, *Chemical Reviews*, 119, 6670-6768 (2019). 99 pp.

**GENERAL READERSHIP PUBLICATIONS**

- G1. J.W. Evans, “Epitaxial Thin Film Growth”, \*SIAM NEWS, November (2010), p.4.  
\*Newsjournal of the *Society for Industrial & Applied Mathematics (SIAM)*.
- G2. D.A. Chen, A. Lii-Rosales, and J.W. Evans,\* Preface: Special Collection commemorating the career of Pat Thiel, *J. Vac. Sci. Technol. A*, 40, 031601 (2022), 2 pp. <https://doi.org/10.1116/6.0001807>

**SUBMITTED**

Da-Jiang Liu, Jie Zhang, Long Qi, and James W. Evans, Molecular simulation using transfer-learned potentials for the disordered nanoscale structure of nitrogen-doped nanoporous carbons, to *Carbon*

T. Ash, Y. Han, J.W. Evans, T.L. Windus, DFT Investigation of the Impact of Inner-Sphere Water Molecules on RE Nitrate Binding to Internal Pore and External Surfaces of MCM-22, to *Phys. Chem. Chem. Phys.*

**BOOKS, CHAPTERS**

1. D. K. Hoffman and J. W. Evans, "The Quantum Statistical Mechanics of Reactive Fluids", in "Few-Body Methods: Principles and Applications," pp. 661-688, edited by T. K. Lim, C. G. Bao, D. P. Hou and H. S. Huber (World Scientific, Singapore, 1986), pp. 661-688.
2. J. W. Evans and M. Sabella, "Mean-Field, Lattice-Gas, and Hybrid Treatments of the Monomer-Dimer Surface Reaction," in "Trends in Statistical Physics", Vol. 1 (Council of Scientific Information, Trivandrim, India, 1994), pp. 107-120.
3. J. W. Evans, "Random and Cooperative Sequential Adsorption: Exactly Solvable Models on 1D Lattices, Continuum Limits, and 2D Extensions", in "Nonequilibrium Statistical Mechanics in One Dimension", edited by V. Privman (Cambridge UP, Cambridge, 1997), pp. 205-227.
4. J.W. Evans and M.C. Bartelt, "Submonolayer Island Formation & Subsequent Multilayer Kinetic Roughening during Metal(100) Homoepitaxy: Fe, Ag & Cu", in "Surface Diffusion: Atomistic & Collective Processes", NATO ASI M.C. Tringides, Ed. (Plenum, New York, 1997), pp. 197-208.
5. J.W. Evans and M.C. Bartelt, "Submonolayer Nucleation and Growth of 2D Islands and Multilayer Mound Formation during Homoepitaxy" in "Morphological Organization in Epitaxial Growth & Removal", Z. Zhang, M.G. Lagally, Ed. (World Scientific, Singapore, 1998), pp. 50-72
6. P.A. Thiel and J.W. Evans, "Cluster Diffusion, Coalescence, and Coarsening in Metal(100) Homoepitaxial Systems" in "Morphological Organization in Epitaxial Growth and Removal", Z. Zhang, M.G. Lagally, Ed. (World Scientific, Singapore, 1998), pp. 384-402.
7. J.W. Evans and M. Tammaro, "Chemical Diffusion, Wave Propagation, and Equistability in Lattice-Gas Models for Bistable Surface Reactions", in "Computer Simulation Studies in Cond. Matter Physics XI", ed. D.P. Landau, H.B. Schuettler (Springer, Berlin, 1999), pp. 103-117.
8. K.J. Caspersen and J.W. Evans, "Realistic Atomistic Models for Mound Formation during Multilayer Growth: Metal(100) Homoepitaxy", Proceedings of the NATO ARW on "Atomistic Aspects of Epitaxial Growth", Corfu, Greece June 2001, edited by M. Kotrla, N.I. Papanicolau, D.D. Vvedensky, and L.T. Wille (Kluwer, Dordrecht, 2002), pp. 197-206.
9. K.J. Caspersen, Da-Jiang Liu, M.C. Bartelt, C.R. Stoldt, A.R. Layson, P.A. Thiel, and J.W. Evans, "Nanostructure Formation and Relaxation in Metal(100) Homoepitaxial Thin Films: Atomistic and Continuum Modeling", in "Computational Materials Chemistry: Methods and Applications", edited by Mark Gordon and Larry Curtiss (Kluwer, Dordrecht, 2004), p. 91-124.
10. J.W. Evans, "Kinetic Monte Carlo Simulation of Non-Equilibrium Lattice-Gas Models: Basic and Refined Algorithms applied to Surface Adsorption Processes", in Handbook of Materials Modeling, Part A, edited by S. Yip (Springer, Berlin, 2005), Ch. 5.12, pp. 1753-1768.
11. J.W. Evans, P.A. Thiel, and Maozhi Li, "KMC Simulation of Epitaxial Thin Film Growth: Formation of Submonolayer Islands & Multilayer Mounds", in "Perspectives on Inorganic, Organic, & Biological Crystal Growth," 13<sup>th</sup> Int. Summer School on Crystal Growth, M. Skowronski, J.J. DeYoreo, C.A. Wang, ed.s (AIP Conf. Proc. Vol. 916, AIP, 2007) pp. 191-211.
12. J.W. Evans, Y. Han, B. Unal, M. Li, K.J.Caspersen, D. Jing, A.R. Layson, C.R. Soldt, T. Duguet, and P.A. Thiel, "From initial to late stages of epitaxial thin film growth: STM analysis and atomistic or coarse-grained modeling", in "Selected Topics on Crystal Growth", M. Wang, K. Tsukamoto, D. Wu, ed.s. Proc. ISSCG14 (AIP Conf. Proc. Vol. 1270, AIP, 2010), pp. 26-44.
13. A. Garcia, C.-J. Wang, D.M. Ackerman, M.S. Gordon, I.I. Slowing and J.W. Evans, Anomalous Kinetics of Catalytic Conversion Reactions in Linear Nanopores mediated by Inhibited Transport: Multiscale Modeling, Chapter 7 in "Chemical Kinetics beyond the Textbook" (World Scientific, Singapore, 2020), pp. 173-190. Ed. K. Lindenberg, R. Metzler, and G. Oshanin.

**REFEREED CONFERENCE PROCEEDINGS**

1. S.-L. Chang, D. E. Sanders, J. W. Evans and P. A. Thiel, "Surface Structures Determined by Kinetic Processes: Adsorption and Diffusion of Oxygen on Pd(100)," in "The Structure of Surfaces II," edited by J. F. van der Veen and M. A. Van Hove (Springer Series in Surface Science, Vol. II, 1988), pp. 231-237.
2. J. W. Evans, "Characterizing the Evolution of Non-Equilibrium Structure during Adsorption", in "The Structure of Surfaces III," edited by S. Y. Tong, M. A. Van Hove, K. Takayanagi and X. D. Xie (Springer Series in Surface Sciences, Vol. III, 1991), pp. 49-54.
3. D. E. Sanders and J. W. Evans, "Downward Funneling Model of Low-Temperature Epitaxial Growth: A Hybrid Molecular Dynamics (MD)-Monte-Carlo (MC) Study," *ibid.* (Springer Series in Surface Sciences, Vol. III, 1991), pp. 38-43.
4. H. C. Kang, P. A. Thiel, and J. W. Evans, "Dependence of Cluster Diffusivity on Cluster Structure," *ibid.* (Springer Series in Surface Sciences, Vol. III, 1991), pp. 55-59.
5. M. C. Bartelt, M. C. Tringides, and J. W. Evans, "Irreversible Island Formation during Deposition: Island Size and Separation Distributions," in "Evolution of Surface and Thin Film Microstructure" edited by H. A. Atwater, E. Chason, M. H. Grabow, and M. G. Lagally, MRS Proceedings, Vol. 280 (MRS, Pittsburgh, 1993), pp. 363-366.
6. M. C. Bartelt and J. W. Evans, "Nucleation and Growth Model for Metal-on-fcc(100) Metal Epitaxy," in "Common Themes and Mechanisms of Epitaxial Growth" edited by P. Fuoss, J. Tsao, D. W. Kisker, A. Zangwill, T. Kuech, MRS Proceedings, Vol. 312 (MRS, Pittsburgh, 1993), pp. 255-260.
7. J.-M. Wen, J. W. Evans, S.-L. Chang, J. W. Burnett, and P. A. Thiel, "Surface Diffusion of Large Ag Clusters on Ag(100)", in "Evolution of Thin-Film and Surface Structure and Morphology", edited by B. G. Demczyk, E. D. Williams, E. Garfunkel, B. M. Clements, and J. E. Cuomo, MRS Proceedings, Vol. 355 (MRS, Boston, 1995), pp.15-20.
8. M.C. Bartelt and J.W. Evans, "Kinetic Roughening of Fe/Fe(100) Epitaxial Thin Films" in "Evolution of Epitaxial Structure and Morphology", edited by A. Zangwill, D. Jesson, D. Chambliss, and R. Clarke, MRS Proceedings, Vol. 399 (MRS, Pittsburgh, 1996), pp.89-94.
9. M.C. Bartelt and J.W. Evans, "Exact Scaling form for the Island Size Distribution in Submonolayer Epitaxial Growth", in "Structure and Evolution of Surfaces", edited by R.C. Cammarata, E.H. Chason, T.L. Einstein, E.D. Williams, MRS Proc. Vol. 440 (MRS, Pittsburgh, 1997), pp.247-252.
10. M.C. Bartelt, J.W. Evans, A.K. Schmid, and R.Q. Hwang, "Island Size and Environment Dependence of Adatom Capture: Cu/Co Islands on Ru(0001)", in "Mechanisms and Principles of Epitaxial Growth in Metallic Systems", edited by L.T. Wille, C.P. Burmester, K. Terakura, G. Comsa, and E.D. Williams, MRS Proceedings, Vol. 528 (MRS, Pittsburgh, 1998), pp. 253-260.
11. K.J. Caspersen, C.R. Stoldt, P.A. Thiel, and J.W. Evans, "Modeling of Metal(100) Homoepitaxial Growth at Very Low Temperatures", in "Recent Developments in Oxide and Metal Epitaxy: Theory and Experiment", edited by M. Yeadon, S. Chiang, R.F.C. Farrow, J.W. Evans, and O. Auciello, MRS Proceedings 619 (MRS, Pittsburgh, 2000), pp. 49-54.
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 Proc. 619 (MRS, Pittsburgh, 2000), pp.173-178.
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.

14. 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.
15. J.W. Evans, Maozhi Li, and M.C. Bartelt "Rate Equation Theory for Island Sizes and Capture Zone Areas in Submonolayer Deposition: Realistic Treatment of Spatial Aspects of Nucleation", MRS Proceedings 749 on "Morphological and Compositional Evolution of Thin Films", edited by M.J. Aziz, N.C. Bartelt, I. Berbezier, J.B. Hannon, and S.J. Hearne (MRS, Pittsburgh, 2003), W.2.2.1-6.
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.
18. 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.
19. D. Jing, Y. Han, B. Unal, J.W. Evans, and P.A. Thiel, "Formation of irregular Al islands by room-temperature deposition on NiAl(110)", MRS Symp. Proc. Vol. 1318. Fall 2010 Symposium UU: "Real-time studies of evolving thin films and interfaces" and Symposia SS/TT/VV (MRS, Pittsburgh, 2011) DOI: 10.1557/opl.2011.484
20. J. Wang, D. Ackerman, K. Kandel, I.I. Slowing, M. Pruski, and J.W. Evans, "Conversion reactions in surface-functionalized mesoporous materials: Effect of restricted transport and the catalytic site distribution", MRS Symp. Proc. Vol. 1411. Fall 2011 Symposium RR (MRS, Pittsburgh, 2012) DOI: 10.1557/opl.2012.229
21. Y. Han and J.W. Evans, "Atomistic modeling of alloy self-growth by vapor deposition: Ni and Al on NiAl(110)", MRS Symp. Proc. Vol. 1411. Fall 2011 Symposium EE (MRS, Pittsburgh, 2012) DOI: 10.1557/opl.2012.761
22. D.-J. Liu, D.M. Ackerman, X. Guo, M.A. Albao, L. Roskop, M.S. Gordon, and J.W. Evans, "Morphological evolution during growth and erosion on vicinal Si(100) surfaces: From electronic structure to atomistic and coarse-grained modeling", MRS Symp. Proc. Vol. 1411. Fall 2011 Symp. EE (MRS, Pittsburgh, 2012) DOI: 10.1557/opl.2012.437
23. J.W. Evans, P.A. Thiel, and B. Unal, "Atomistic and coarse-grained modeling strategies for thin film nucleation and growth on quasicrystalline surfaces", MRS Symp. Proc. Vol. 1517 (MRS, Pittsburgh, 2013) DOI: 10.1557/opl.2012.1753
24. Y. Han, A.K. Engstfeld, C.Z. Wang, L.D. Roelofs, R.J. Behm, and J.W. Evans, "Atomistic modeling of Ru NC formation on graphene/Ru(0001): Thermodynamic vs. kinetic directed assembly", MRS Symp. Proc. Vol. 1498 (MRS, Pittsburgh, 2013) DOI: 10.1557/opl.2013.106
25. Jing Wang, Andrés Garcia, David M. Ackerman, Mark S. Gordon, Igor I. Slowing, Takeshi Kobayashi, Marek Pruski and James W. Evans, Multi-functionalization of nanoporous catalytic materials to enhance reaction yield: Statistical mechanical modeling for conversion reactions with restricted diffusive transport, MRS Symp. Proc. Vol. 1641 (MRS, Pittsburgh, 2014) DOI: <http://dx.doi.org/10.1557/opl.2014.321>.

**INVITED PAPERS, TALKS. SEE APPENDED LISTING:** Total ~190 (to 08/2024)

**CONTRIBUTED PAPERS, TALKS. SEE APPENDED LISTING:** Total ~ 99

### **HONORS AND AWARDS**

Fellow, American Physical Society – Division of Condensed Matter Physics (2002)

ISU/LAS Mid-Career Achievement in Research (2005)

Elsevier “Surface Science Reports: Top Cited Article 2005-2010” (#2 in 2005-10)

Elsevier “Progress in Surface Science” Highly-cited research (Dec. 2016)

American Physical Society (APS) Outstanding Referee (2015)

### **PROFESSIONAL INVOLVEMENT**

Editorial Board, Nanomaterials (MDPI), 2020-present

Editorial Board, Surface Science (Elsevier) 2015-present

Editorial Board, Computational Materials Science (Elsevier) 2014-2017

Editorial Board, Journal of Chemical Physics (American Institute of Physics) 2013-2015

SIAM Materials Science Activity Group Nominating Committee 2013.

Nominator for APS Fellows: 2010 and 2011 (both successful).

### **CONFERENCE & SYMPOSIUM ORGANIZATION/ REVIEW PANELS**

\*Lead organizer: SIAM 2021 Materials Science Minisymposium: Nanocrystals and epitaxial nanoclusters: Self-assembly, structure and stability. On-line, May (with Kristen Fichthorn, PSU)

\*Lead Organizer: SIAM 2018 Materials Science Minisymposium: Aggregation, Growth, and Coarsening, Portland OR, July (with Bob Pego CMU)

\* Co-Organizer, NSF Ki-Net Workshop Kinetic Descriptions of Chem & Bio Systems (2017) with H Liu

\*Lead-organizer: SIAM Materials Science 2016 Minisymposium on “Mesoscale Modeling of Materials and Processes” Philadelphia (with P. Plechac and D. Margetis).

\*Co-organizer: NSF-supported Ki-Net 2014 Summer School on “Dynamics and numerics of non-local PDE’s and related equations with applications in the physical and biological sciences” (with H Liu)

\*Co-organizer: ISU LAS symposium on Complex Materials (2014)

\*Lead-organizer: SIAM 2013 Materials Science Conference Mini-symposium on “Morphological evolution of surfaces, thin films, and clusters”. Philadelphia Co-organizers: D. Margetis

\*Lead-organizer: AMS 2013 Sectional Meeting Symposia on “Stochastic processes with applications to physics...” Ames, ISU, April 2013 (with A. Roiterstein, A. Ghosh, J. Peterson)

\*Co-organizer: AMS 2013 Sectional Mtg Symp. on “Kinetic & Hydrodynamic PDEs” (with Liu, Tadmor)

\*Co-organizer: 2013 NSF Mathematical Sciences-supported Ki-Net Workshop on “Kinetic PDE’s: Analysis and Computation”, Ames ISU April 2013 (with Hailiang Liu, Eitan Tadmor)

\*Lead organizer: 2012 SIAM Annual Meeting Mini-symposium: “Surface and thin film evolution: self-assembly, instability, pattern formation”. (June 2012, Minneapolis) Co-organizer: D. Margetis

\*Co-organizer: 2010 CSCAMM – U. Maryland Workshop on “Non-equilibrium interface and surface dynamics: theory, experiment, and simulation from atomistic to continuum scales”. University of Maryland. Co-organizers: J. Weeks, T. Einstein, R. Phaneuf, D. Margetis

\*Lead-organizer: SIAM 2010 Materials Science Conference Mini-symposium on “Growth and Relaxation of Epitaxial Thin Films”. Philadelphia Co-organizers: D. Margetis and P. Smereka

\*Co-organizer: 2009 IMA Symp. on “Spatiotemporal Reaction-Diffusion Phenomena”, with Arnd Scheel.



- \*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.
- \*Lead-organizer of NSF-IMA co-sponsored ISU/Ames Lab Workshop on “Computational and Mathematical Aspects of Materials and Fluids” with Hailiang Liu, April 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: Fall 2004 MRS Meeting Symp JJ on "Modeling of Morphological Evolution at Surfaces & Interfaces". 3.5 days (91 presentations) in memory of Maria C. Bartelt (Scientific Leader, Comp. Mat. Sciences, CMS, 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 APS (Div. Materials Physics) 2003 March Meeting Focus Session on “Morphological Evolution of Nanostructures, Interfaces, Surfaces, Thin Films” with R. Phaneuf, R. Hwang, 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.

**REFEREE FOR THE FOLLOWING JOURNALS:**

Science	Physical Review Letters	Chaos	New J. Physics
J. Mathematical Physics	J. Chemical Physics	J. Crystal Growth	Physica D
J. Statistical Physics	Physical Review B	Physica A	Appl Phys Lett
Physical Chemistry	Physical Review E	Chemical Physics	Nanotech.
Langmuir	Surface Science	J. Colloids and Surfaces A	
Theoretical Chimica Acta	Physics Letters A	Vacuum	J. Appl. Phys.
Applied Physics A	Europhysics Letters	J. Catalysis	Thin Solid Films
J. Vacuum Science & Tech.	Chemical Physics Letters	J. Energetic Materials	MRS Proc.
Euro. J. Physics B	Chem. Eng. Science	Surface Coatings & Tech.	
J. Low Temp. Physics	Adv. Applied Prob.	Discrete Contin. Dyn. Sys. B	
Philosophical Magazine	Canada J. Physics	J. Zhejiang U. Sci. A	

**LEVEL OF RECENT JOURNAL PAPER AND PROPOSAL REVIEWING ACTIVITY:**

**1992:** 17 journal papers; **1993:** 15 journal papers, 1 proposal.  
**1994:** 19 journal papers, 2 proposals, 1 tenure case; **1995:** 18 journal papers, 2 NSF ppls.  
**1996:** 19 journal/proceedings papers, 4 proposals, 1 promotion case.  
**1997:** 23 journal papers, 5 proposals, 2 award nom.; **1998:** 21 journal papers, 1 proposal;  
**1999:** 23 journal papers, 2 proposals, 1 tenure case. **2000:** 15 journal papers, 1 NSF proposal.  
**2001:** reviewed 23 journal papers, 2 NSF proposals, 1 DOE proposal, 1 award nomination.  
**2002:** reviewed 20 journal papers, 3 NSF +1 DOE +1 Research Corp. proposal, 2 tenure cases  
**2003:** 27 journal papers, 1 NSF, 1 DOE proposal, 1 promotion; **2004:** 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 22 journal papers, 1 NSF Career.  
**2009:** reviewed 24 journal papers, 2 NSF, 1 Czech Sci. Fdn.  
**2010:** reviewed 18 journal papers, 1 NSF ppl, 1 Czech Sci. Fdn. Ppl.  
**2011:** reviewed 25 journal papers, 3 NSF ppl, 1 Norway ppl.  
**2012:** reviewed 27 journal papers, 1 NSF ppl, 3 DOE ppl.  
**2013:** reviewed 29 journal papers  
**2014:** reviewed 29 journal papers, 2 NSF ppl.  
**2015:** reviewed 30 journal papers, 2x DOE ppl, 10 senior DOE senior nominations  
**2016:** reviewed 19 journal papers and 3 DOE proposals  
**2017:** reviewed 30 journal papers  
**2018:** reviewed 23 journal papers to date, and 1 DOE proposal, 1 tenure case.  
**2019:** reviewed 26 journal papers, and 2 DOE BES proposals.  
**2020:** reviewed 17 journal papers  
**2021:** reviewed 20 journal papers; plus handled 5 reviews for Nanomaterials;  
 reviewed 8 applicants for high-profile DOE scientific award  
**2022:** reviewed 10 journal papers; handled 13 reviews for Nanomaterials  
**2023:** reviewed 9 journal papers; handled 13 reviews for Nanomaterials; 1 DOE review  
**2024:** reviewed 6 journal papers + 2 for Nanomaterials to date; provided 2 promotion letters

**REVIEWER FOR THE FOLLOWING FUNDING AGENCIES:**

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

**FUNDED PROPOSALS****CURRENTLY EXTERNALLY FUNDED RESEARCH PROJECTS AS PI OR CO-PI:**

Title: Computational & Theoretical Chemistry: Elucidating interplay between non-equilibrium adsorption, transport, separation, and reaction processes in complex environments...  
Source of Support: USDOE Basic Energy Sciences – Chemical Sciences Division, CTC program  
Lead Principal Investigator: T.L. Windus; co-PIs: J.W. Evans, M.S. Gordon, D.-J. Liu  
\*Amount & Period: ~\$3,000,000 for 10/2023-09/2026 with ~\$1,080,000 to Evans.

Title: Development of exascale software for heterogeneous and interfacial catalysis  
Source of Support: USDOE Basic Energy Sciences – Chemical Sciences Division  
Lead Principal Investigator: M.S. Gordon; co-PI's: J.W. Evans, T. Windus and ~8 others  
\*Amount & Period: ~\$4,200,000 for 10/2018-09/2023 + no cost extension to 9/24 with ~\$200,000 to Evans

Title: Geo-inspired Separation of Rare Earth Elements  
Source: USDOE Basic Energy Sciences – Chemical Sciences Division  
Lead Principal Investigator: T. Prozorov; Co-PIs: J.W. Evans, I.I. Slowing/W. Huang, and 4 others  
\*Amount & Period: ~\$2.9M for 10/2021-9/2024 + carryover funding to 9/25 with ~\$240,000 to Evans

**CURRENTLY EXTERNALLY FUNDED RESEARCH PROJECT AS COLLABORATOR:**

Title: Surface structures far-from-equilibrium  
Source of support: USDOE Basic Energy Sciences – Materials Sciences  
Principal Investigator: M. Tringides; Co-PIs: P.A.Thiel, C.Z. Wang et al. Collaborator: J.W. Evans  
\*Amount and period: 10/2021-9/2024 with \$165,000 to support Evans-group Scientist Yong Han

**PENDING PROPOSALS OR PRE-PROPOSALS:**

None

**RECENTLY INTERNALLY FUNDED RESEARCH PROJECTS AS PI OR CO-PI:**

Title: Control of structure and composition of functional nanoclusters  
– an integrated experimental and modeling approach  
Source of Support: Presidential Interdisciplinary Research Initiative (PIRS)  
Principle Investigator: J.W. Evans Co-PIs: W. Huang, J. Vela  
\*Amount & Period: \$50,000 for 07/2017 - 09/2019 with \$18,000 to Evans.

**SEE BELOW FOR PREVIOUSLY FUNDED EXTERNAL PROPOSALS**

**PREVIOUSLY FUNDED NSF PROJECTS AS PI OR CO-PI:**

Title: Environment-dependent coarsening of supported metallic nanoclusters (CHE-1507223)

Source of Support: NSF Chemistry Division: Chemical Dynamics Program

Principle Investigator: P.A. Thiel; Co-PI: J.W. Evans

Amount & Period: \$385,000 for 08/2015 - 08/2020 with \$170,000 to Evans.

Title: Formation and Stability of Supported Metal Nanostructures (CHE-1111500)

Source of Support: NSF Chemistry Division: Chemical Dynamics Program

Principle Investigator: P.A. Thiel; Co-PI: J.W. Evans

Amount & Period: \$500,000 for 07/2011 - 06/2016 with \$250 K to Evans.

Title: Assembly and stability of metal nanostructures on surfaces (CHE-00809472)

NSF Analytical/Surface Chemistry

Principle Investigator: J.W. Evans; Co-PI: P.A. Thiel

Amount & Period: \$594,000 with \$280,000 for Evans (5 yr total) for 07/15/2008 - 06/30/2011

Title: Spatial Organization in Epitaxial Thin Films and Chemisorbed Layers: Manipulation of Nano- and Meso-scale Structure on Metal Substrates (CHE-0414378) NSF 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 08/01/2004 - 07/31/2009

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.

**PREVIOUSLY FUNDED NSF REU PROJECTS AS CO-PI:**

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.

**PREVIOUSLY FUNDED USDOE-BES PROJECTS AS PI OR CO-PI:**

Title: Theoretical & Computational Tools for Modeling of Energy Relevant Catalysis on Multiple Scales

Source of Support: USDOE Basic Energy Sciences – Chemical Sciences Division, CTC program

Lead Principal Investigator: J.W. Evans; co-PIs: M.S. Gordon, K. Ruedenberg, T. Windus

\*Amount & Period: ~\$3,512,000 (6 year total) for 10/2017-09/2023 with ~\$1,630,000 to Evans.

Title: Theoretical & Computational Tools for Modeling of Energy Relevant Catalysis on Multiple Scales  
Source of Support: USDOE Basic Energy Sciences – Chemical Sciences Division, CTC program  
Lead Principal Investigator: J.W. Evans; co-PIs: M.S. Gordon, K. Ruedenberg, T. Windus  
\*Amount & Period: ~\$1,760,000 (3 year total) for 10/2014-09/2017 with ~\$870,000 to Evans.

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; co-PI's: K. Ruedenberg, T. Windus  
Amount & Period: ~\$2,000,000 for 10/2010-09/2014 with \$740K to Evans

Title: Theoretical and Computational Tools for Modeling of Energy-Relevant Catalysis  
Source of Support: USDOE BES Chemical Sciences  
Principal Investigators: J.W. Evans and M.S. Gordon  
Amount & Period: \$500,000 from 09/01/2010 to 09/30/2014 (\$250K to Evans)

Title: Selective and Efficient Catalysis in 3D Controlled Environments  
Source of Support: USDOE Basic Energy Sciences, Division of Chemical Sciences  
PI: M. Pruski; Co-PI's: A. Bakac, J. Evans, A. Sadow, I. Slowing, J. Vela  
Amount & Period: ~\$600,000 with ~\$75K for Evans for 10/1/2010-09/30/2013

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: ~\$345,000 per annum for 10/07-09/10 (~\$164K in FY09, \$138K in FY10 for Evans).

Title: Selective and Efficient Catalysis in 3D Controlled Environments  
Source of Support: USDOE Basic Energy Sciences, Division of Chemical Sciences  
PI: V.-S.Y Lin, co-PI's: M. Pruski; CoPI's: A. Bakac, A. Sadow, J. Evans  
Amount & Period: ~\$600,000 with ~\$15K 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) (no significant funding to Evans) for 10/01/08 to 09/30/11

Title: A Multi-Scale Approach to the Simulation of Lignocellulosic Biomass  
Source of Support: USDOE SciDAC  
Principal Investigators: J.C. Smith (ORNL), M. Gordon. Co-PI's: T. Windus, M. Lamm, J. Evans  
Amount & Period: \$1,800,000 (3 year total) (no support used by Evans) from 10/01/08 to 09/30/11

Title: High-Performance Comp. Chem.: Scalable Electronic Structure Theory, Non-Equil Stat Mech,...  
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: 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

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 for several years 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: M. Gordon; 4 Co-PI's; several senior collaborators (incl. Evans). Amount & Period: ~\$400,000, 2001.

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.

**APPENDIX: Invited Papers, Talks (total ~ 188)****2024**

1. Atomistic-level stochastic modeling & KMC simulation of metal nanocrystal evolution with ab-initio guided kinetics: Reshaping and intermixing, International Workshop on Modeling of Crystal Growth , Timisoara Romania September 2024 (\$2,500 NSF travel support)

**2023**

1. Nucleation-mediated processes for metal nanoclusters, Gordon Research Conference on Crystal Growth and Assembly, Southern NH U June
2. Evolution of catalytic metal nanoclusters, Great Plains Catalysis Society Webinar Series, July
3. Reshaping and diffusion of metal nanocrystals, 23<sup>rd</sup> American Assoc Crystal Growth Mtg, Tuscon Aug

**2022**

1. Formation & coarsening of metal nanostructures surfaces, Physical Electronics Conf, Loyola U June
2. Shape stability of fcc metal nanocubes and octahedra, Gordon Research Conference on Nobel Metal Nanoparticles, Mt Holyoak MA June
3. Assembly & stability of supported metal nanoclusters, 86<sup>th</sup> AVS International Symposium, Pittsburg

**2021**

1. Catalytic reaction-diffusion processes in nanoporous materials, Louisiana State U ChemE, February
2. Self-assembly and stability of metal nanoclusters, Louisiana State U, Physics, April
3. Reshaping of metallic nanocrystals, SIAM Materials Science Meeting (on-line), hosted by Basque Center for Applied Math (Spain), June
4. Formation and stability of supported metal nanoclusters, AVS Symposium – canceled due to Covid, November

**2020**

1. Statistical mechanical and coarse-grained modeling of catalytic systems, DOE Computational Theoretical Chemistry Virtual Meeting, July.

**The following were cancelled due to covid-19:**

2. Modeling of metal nanoclusters adsorbed on and intercalated beneath the surface of layered materials, SIAM MS20 Symposium on ‘Modeling and simulation of 2D materials and ultrathin films, Bilbao Spain May
3. Atomistic modeling of diffusion of 2D and 3D epitaxially supported nanoclusters, SIAM MS20 Symposium on ‘Modeling of metal nanoclusters adsorbed on and intercalated in layered materials’ Bilbao Spain May
4. Lecture series covering 4+ topics: (i) Self-assembly and stability of nanomaterials; (ii) Initial stages of thin film growth: nucleation theory; (iii) Multilayer thin film growth and kinetic roughening; (iv) Coarsening processes in thin films; (v) Shape stability of 3D Nanocrystals, Sichuan U, China, July
5. Gordon Research Conference on Noble Metal Nanoparticles, Discussion Leader, June

**2019:**

1. Assembly and stability of nanoclusters on surfaces, Erwin Schroedinger Inst., Vienna, Austria Nov.
2. Modeling of chemisorption and catalysis on metal surfaces and in mesopores, TU Wien, Nov.

**2018:**

1. Kinetics of nucleation and growth of intercalated islands, International Conference of 2D Quantum Materials, Snowbird Utah, March.
3. Modeling non-equilibrium nanocluster growth shapes in surface systems, SIAM MS18 Symposium on Models & mechanisms of nanoscale crystal growth, Portland OR July
2. Formation and coarsening of nanoclusters on surfaces, SIAM MS18 Symposium on Aggregation, Growth and Coarsening, Portland OR July
4. Novel nanoscale cluster dynamics on surfaces, Int. Center for Math. Sci. conference on ‘Particle based methods in materials science’, Edinburgh, Scotland, July
5. Assembly and stability of structures in the nanoworld, Physics, Gustavus Adolphus University, Nov.

**2017:**

1. Predictive atomistic-level modeling of self-assembly and catalysis on metal surfaces, Chemical Engineering, LSU, Baton Rouge, March.
2. Non-equilibrium correlations in reaction-diffusion models with inhibited stirring, NSF KI-Net conference on “Kinetic Modeling of chemical and biological systems”, ISU, March
3. From atomistic to continuum modeling of cooperative processes, Truman State U, Missouri, April
4. Statistical mechanical and energetic analysis of chemisorption and catalysis on metals, Computational & Theoretical Chemistry USDOE PI Meeting, Washington DC, April.
5. Predictive atomistic-level modeling of diffusion-mediated self-assembly and catalytic reaction processes on metal surfaces, 8<sup>th</sup> Int. Workshop on Surface Physics, Trzebnica, Poland June
6. Self-assembly and stability of metal nanoclusters, Plenary talk at Nano@IAState, July.

**2016:**

1. “Formulations treating stochastic effects in thin film growth and relaxation including contributions from Peter Smereka”, Symposium on Analysis Modeling and Simulation of Materials in Memory of Peter Smereka, SIAM Conf. on Math Aspects of Mat Sci. Philadelphia May 2016
2. “Coarse-grained mesoscale modeling for deposition-diffusion and reaction-diffusion systems”, Symp on Mesoscale Modeling of Non-equilibrium Assembly, Transport & Reaction Processes, SIAM MS16.
3. “Coarse-graining from atomistic to continuum models for island and step dynamics...” Symposium on Microscopic Processes and Non-equilibrium Phenomena in Epitaxial Growth, SIAM MS16

**2015:**

1. “Non-equilibrium statistical mechanical & coarse-grained mesoscale modeling of catalytic reaction-diffusion processes” Computational & Theoretical Chemistry USDOE PI Meeting, Annapolis MD April.
2. "KMC simulation of molecular-level models with ab-initio energetics & coarse-grained mesoscale descriptions of catalytic surface reactions" Washington State University, Department of Chemical & Bio Engineering, Pullman, Oct.
3. “Nucleation & growth of nanoclusters during surface deposition: Spatial aspects on nucleation and ab-initio treatment of growth kinetics”, U. Science & Technology China (USTC), Hefei, China December

**2014:**

1. Drake U, Predictive modeling of complex self-assembly and pattern-forming processes. March
2. NSF Ki-Net Summer School: Fragmentation of capture zones. May
3. NSF Ki-Net Summer School: Discrete non-local models for phase transitions. May
4. SIAM annual meeting: Self-assembly and stability of 2D nanoclusters. Chicago July
5. IUVSTA Int. Workshop: Self-assembly and stability of bimetallic nanoclusters Eisenerz Austria Sept.
6. U. Delaware Applied Mathematics Colloquium, November

**2013:**

1. “From stochastic Interacting Particle Systems to lattice differential equations for reaction-diffusion systems”, NSF-supported Inst. Math & its Applications, U. Minnesota (April 2013)
2. NSF Math. Sci. –supported Ki-Net Workshop on “Kinetic PDE’s” (Ames, April 2013)
3. Symposium of “Kinetic and Hydrodynamic PDE’s”, AMS Sectional Meeting, April 2013.
4. “Unstable multilayer homoepitaxial growth: From 2D islands to 3D mounds”  
Symposium on “Epitaxial Thin Film Growth”, SIAM Materials Science Conference, June 2013.
5. “Nanocluster self-assembly: Far-from-equilibrium shapes and composition profiles”,  
Symposium on “Morphological evolution of crystalline surface, thin films, and nanoclusters” (self-invite as organizer), SIAM Materials Science Conference, June 2013.



**2012:**

1. "Self-assembly of Epitaxial Metal Nanostructures", Nanoscience Program, Arizona State U., Jan.
2. "KMC simulations of atomistic lattice-gas models for surface processes", Arizona State U., Jan.
3. "Predictive modeling of the formation of binary alloy nanostructures", ICREM-Brown U workshop on "Heterostructured nanocrystalline materials", Brown University, Providence, RI May.
4. "Multi-site lattice-gas modeling of the far-from-equilibrium formation of epitaxial nanostructures", U. Minn. Symposium on "Advancing QChem: Interfacing electronic structure with dynamics", June.
5. "Capture zones for submonolayer island formation during deposition", SIAM mini-symposium on "Surface and thin film evolution" (self-invite as organizer), Minneapolis, MN, July.
6. "Self-assembly of single- and multi-component epitaxial metal nanostructures" U. Florida Department of Materials Science, Gainesville, FL, August.
7. "Formation on multicomponent epitaxial nanostructures by self-assembly and directed assembly", IPAM-UCLA workshop on "Atomistic and mesoscale modeling of materials defects", October.
8. "Statistical Mechanical/multiscale modeling of reaction systems", DOE Chem. Sci CPIMS Mtg, Oct.

**2011:**

1. "Far-from-equilibrium growth of epitaxial metal nanostructures in multi-component systems: predictive atomistic modeling", CMSN Coordinating Meeting, Dallas Texas, January
2. "Atomistic and Coarse-Grained Modeling of Epitaxial Thin Film Growth and Relaxation", Illinois Institute of Technology, Chicago, March.
3. "Interface Propagation: From discrete stochastic models to PDE's", IA PDE conference, Ames, May
4. "Far-from-equilibrium growth of epitaxial metal nanostructures in multi-component systems: predictive atomistic modeling", ACCGE18, Monterey, August.

**2010:**

1. "Stochastic Models for Spatial Epidemics", Spring Central AMS Regional Mtg, St. Paul, April 2010.
2. "Predictive Atomistic and Coarse-Grained Modeling of Epitaxial Thin Film Growth", Plenary lecture at SIAM Materials Science Conference, May 2010.
- \*3. "Interplay of spatial organization and ordering in the growth of alloy films", Minisym on Growth & Relaxation of Epitaxial Thin Films, SIAM Mat. Sci. Conf., May 2010. \*self-invite as symp co-organizer
4. "Novel coarsening kinetics for islands on surfaces: Effects of anisotropy, QSE, and additives" Minisym on Self-similarity/scaling in models for materials science, SIAM Mat. Sci. Conf. May 2010.
5. "Atomistic and Coarse-Grained Modeling of Epitaxial Thin Film Growth", Int. Conf. on "Mathematical Aspects of Crystal Growth" Sapporo, Japan July 2010.
6. "Atomistic and Coarse-Grained Modeling of Crystal Growth by Vapor Deposition", 14<sup>th</sup> International Summer School on Crystal Growth, Dalian, China, August 2010.
7. "Modeling Strategies for of Crystal Growth: KMC et al. (Tutorial Lecture)", 14<sup>th</sup> International Summer School on Crystal Growth, Dalian, China, August 2010.
8. "Realistic multi-site multi-component lattice-gas modeling for epitaxial growth of metal films on binary alloy surfaces", Workshop on "Non-equilibrium interface and surface dynamics: Theory, experiment and simulation from atomistic to continuum scales" CSCAMM, U. Maryland, October 2010.

**2009:**

1. "Atomistic and Multiscale modeling of CO-oxidation: From nanoscale fluctuations to mesoscale fronts", Inst Physical Chemistry and Catalysis, U. Ulm, Germany February 2009
2. "Modeling of the Growth of Homoepitaxial & Heteroepitaxial Ag Thin Films: Kinetics, Quantum Size Effects, and Strain", Dept. Physics, U. Ilmenau, Germany February 2009
3. "Modeling of the Growth of Homoepitaxial & Heteroepitaxial Ag Thin Films: Kinetics, Quantum Size Effects, and Strain", Dept. Physics, U. Koeln, Germany February 2009
4. "Statistical Mechanical treatment of Schloegl's Second Model for Autocatalysis", Harz Seminar on Non-linear Dynamics, Harz Mountains, Germany, March 2009

5. "Atomistic and Multiscale modeling of CO-oxidation: From nanoscale fluctuations to mesoscale fronts", Dept. Physical & Electrochemistry, U. Hannover, Germany March 2009
6. "Modeling of the Growth of Homoepitaxial & Heteroepitaxial Ag Thin Films: Kinetics, Quantum Size Effects, and Strain", Inst. Surface Physics, U. Hannover, Germany February 2009
7. "Epitaxial growth of metal films on NiAl(110) binary alloy substrate", Surface Kinetics International conference, U. Utah, March 2009.
8. "Stochastic "interacting particle systems" models for reaction-diffusion systems: Non-linear kinetics, steady-state bifurcations (phase transitions), reaction fronts" IMA Seminar on Mathematics and Chemistry, IMA, U Minnesota, April 2009.
9. "From molecular-level reaction models to continuum reaction diffusion equations", IMA Symposium on Spatiotemporal Reaction-Diffusion Phenomena, IMA U Minnesota, May 2009
10. "Atomistic and multiscale modeling of CO-oxidation on Pd(100) and Rh(100): From nanoscale fluctuations to mesoscale reaction fronts" Institute of Physics-CAS, Beijing, June 2009.
11. "Evolution of Thin Film Morphology during Epitaxial Growth: Modeling and Experiment" Dept. Physics, Renmin University, Beijing, June 2009
12. "Predictive Atomistic and Coarse-Grained Modeling of Epitaxial Thin Film Growth", Workshop on Mathematical modeling in the Materials Science, Inst. Math Science, Nat. U. Singapore, July 2009
13. "Coarsening of Island Distributions on Surfaces: Ostwald vs Smoluchowski vs Anomalous Ripening", Workshop on Math. Modeling in the Materials Science, Inst. Math. Sci., Nat. U. Singapore, July 2009
14. "Nanostructure formation in metal films: Highlights of STM studies and atomistic modeling", Bunsen Colloquium: Microscopic Views on Interface Phenomena, Reisenburg Castle, Germany, December 2009.

**2008:**

1. "Atomistic and multiscale modeling of CO-oxidation", CMSN Coordinating Meeting, Gatlinburg, Tennessee, Oct.31-Nov.1 (2008)
2. "Statistical Mechanical and Multiscale Modeling of Surface Reaction Processes", CPIMS Contractors Meeting, Airlee House, Warrenton, Virginia, Nov. 2008.
3. "Predicting Multilayer Growth Morphologies of Ag Films controlled by Step Edge Barriers & Quantum Size Effects", American Soc. Crystal Growth West Mtg, Fallen Leaf Lake, S. Lake Tahoe, CA June 2008.
- \*4. "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. \*self-invitation as symp. co-organizer
5. "Step dynamics modeling of multilayer growth: Step edge barriers, quantum size effects, & fluctuations" SIAM Conference on "Mathematical Aspects of Materials Science", Minisymp.: Kinetics and Fluctuations of Crystal Surfaces: From Discrete Models to Continuum, Philadelphia May 2008.
6. "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:**

1. "Growth of Ag films on Alloy Substrates", CMSN Coordinating Mtg, Iowa State U., Ames, Oct 2007
2. "Kinetic Monte Carlo Simulation of Epitaxial Thin Film Growth" 13<sup>th</sup> Int. Summer School on Crystal Growth, Park City, Utah, August 2007.
3. "Kinetic Monte Carlo Simulation of Epitaxial Thin Film Growth", Department of Materials Science, U. Utah, August 2007.

**2006:**

1. "Metal film growth on complex substrates: 5-fold surfaces of icosohedral quasicrystals", CMSN Coordinating Meeting, U. Maryland – College Park, October 2006.
2. "Morphological evolution in thin film homoepitaxy: Modeling and experimental studies of unstable multilayer growth" Inst. Materials Research, Tohoku University, Sendai, Japan, June 2006.

3. “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.
4. “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.

**2005:**

1. “Atomistic Modeling of Cooperative Phenomena in Surface Reaction Processes”, USDOE BES Meeting on Condensed Phase & Interfacial Molecular Science, Arlie House, Warrenton, VA, Oct. 2005.
2. “Atomistic Modeling of Cooperative Phenomena in Surface Reactions”, Lawrence Berkeley National Laboratory, Berkeley, October 2005.
3. “Modeling Strategies for Unstable Multilayer Growth: From Atomistic to 2D Continuum Step Dynamics to 3D Continuum”, CMSN Coordinating Meeting, U. Wisconsin – Madison, October 2005.
4. “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.
5. “Integrated Modeling and Experimental Studies of Homoepitaxial Thin Film Growth”, APS Workshop on Surface and Interface Science, Argonne National Laboratory, September 2005.
6. “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
7. “Atomistic and Continuum Modeling Strategies for Homoepitaxial Thin Film Growth”, Institute of Mathematics & Applications, University of Minnesota, Feb. 2005
8. “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)
9. “From Atomic Scale Ordering to Mesoscale Reaction Front Propagation: CO-oxidation on Pd(100)”, Department of Chemistry, National University of Singapore, January 2005
10. “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:**

1. “Formation and Relaxation of Submonolayer Films: Atomistic and Continuum Modeling Approaches”, CNRS UJF – Grenoble, France, Sept. 2004
2. “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
3. “Coarsening Processes in Homoepitaxial Thin Films: Atomistic and Continuum Modeling”, SIAM Conference on Mathematical Aspects of Materials Science, Los Angeles, May 2004.
4. “Predictive Models for Nanostructure Evolution during Epitaxial Thin Film Growth”, March Meeting of the American Physical Society, Monteval, March 2004.

**2003:**

1. “Atomistic and Continuum Modeling of Thin Film Growth and Relaxation” CMSN Proposal Formulation Workshop, Emory University, Atlanta, GA Jan. 2003
2. “Fluctuations and Patterns in Surface Reactions: A Statistical Physics Approach” Conference on Catalysis, Chalmers University, Goteburg, Sweden March 2003.
3. “Comparison of homoepitaxial film growth for Ag/Ag(100) and Ag/Ag(111)”, Kansas State University, Manhattan, Kansas, May 2003.
4. “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:**

1. "Growth & Relaxation of Epitaxial Thin Films: Atomistic & Continuum Modeling", Plenary Talk UCLA IPAM Workshop "Math. in Nanoscale Science", Lake Arrowhead, CA, Dec 2002.
2. "Multilayer Growth of Metal Homoepitaxial Films: Formation and Evolution of Mounds", Ecole des Mines, Nancy, France, June 2002.
3. "Nanostructure Formation and Relaxation in Metal(100) Homoepitaxial Systems", Institute of Surface Physics, Universitaet Hannover, Hannover, Germany, June 2002.
4. "Fluctuations and Reaction Fronts in a Lattice-Gas Model for CO-Oxidation", Department of Physics, Humboldt Universitaet, Berlin, Germany, June 2002.
5. "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.
6. "Interacting Particles Systems Models for Surface Adsorption and Reaction", Department of Mathematics, Monash University, Australia, May 2002.
7. "Formation and Evolution of Mounds during Ag/Ag(100) Growth", Int. Seminar on "Models of Epitaxial Crystal Growth", MPI fuer Physik Complexer Systeme, Dresden, Germany, Mar 2002.
8. "Nanostructure Evolution in Thin Film Growth and Relaxation", Department of Physics, Kansas State University, Manhattan, Kansas, February 2002.

**2001:**

1. "Growth and Relaxation in Submonolayer Epitaxial Films", 26th International Nathiagali Summer College on Physics and Contemporary Needs (INSC), Nathiagali, Pakistan, July 2001.
2. "Multilayer growth of Epitaxial Films: Kinetic Roughening and Mound Formation", 26th INSC, Nathiagali, Pakistan, July 2001.
3. "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.
4. "Multilayer Growth in Metal(100) Homoepitaxy: Key processes in Predictive Atomistic Models", NATO Advanced Research Workshop, Corfu, Greece, June 2001.
5. "Nanostructure Formation and Relaxation in Metal(100) Homoepitaxial Systems", Kamerlingh-Onnes Laboratory, University of Leiden, The Netherlands, June 2001.
6. "Nanostructure Formation and Relaxation in Metal(100) Homoepitaxial Systems", Department of Applied Physics, University of Twente, The Netherlands, June 2001.

**2000:**

1. "Morphological Evolution during Multilayer Growth of Metal Films", for "Computer Simulation in Electrochemistry" Symposium, 220th National ACS Meeting, Washington DC, August 2000.
2. "Simulations of Submonolayer Epitaxy and Etching", *ibid*, Washington DC, August 2000.
3. "Growth and Relaxation of Thin Metal Films", Physics, University of Maryland, August 2000.
4. "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.
5. "Developments in Submonolayer Growth and Relaxation of Homoepitaxial Metal Films", Dipartimento di Fisica, Universita degli Studi di Firenze, Florence, Italy, July 2000.
6. "Ordering, Percolation, and Diffusion in Atomistic Models for Surface Reactions", CECAM Workshop on "Catalysis from First-Principles", Lyon, France, July 2000.
7. "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.

8. "Temperature-Dependence of Multilayer Growth of Ag/Ag(100)", Department of Physical Chemistry, Universitaet Ulm, Germany, June 2000.
9. "Interplay between Ordering, Percolation, and Transport in Disordered Systems", Laboratoire de Science et Genie des Materiaux Metalliques (CNRS), Ecole des Mines, Nancy, France, June 2000.
10. "Multilayer Growth of Ag/Ag(100) Homoepitaxial Thin Films", Bonassola workshop on Nanoscale Modification of Surfaces and Thin Films, Bonassola, Italy, May 2000.

**1999:**

1. "Homoepitaxial Growth at Low Temperatures: Some Surprises for Simple Systems", DOE Workshop on "The Physics of Ultrathin Films near Metal-Insulator Transition", Brown University, RI, Dec. 1999.
2. "Non-Equilibrium Growth and Post-Deposition Relaxation of Epitaxial Thin Films", Physics Colloquium, University of Rhode Island, December 1999.
3. "Spatio-Temporal Behavior in Surface Reactions: Chemical Diffusion, Chemical Waves, and Fluctuations", Sandia National Laboratories, Livermore, California, February 1999.
4. "Growth and Relaxation of Epitaxial Metal Thin Films", Materials Research Laboratory, University of Illinois, Urbana-Champaign, Illinois, January 1999.

**1998:**

1. "Formation and Relaxation of Two-Dimensional Metal Islands on Surfaces", Fall MRS Symposium
2. "Surface and Interface Structure and Dynamics", Boston, December, 1998.
3. "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.
4. "Chemical Diffusion and Wave Propagation in Surface Reactions", Abteilung Physical Chemie, Fritz-Haber-Institute, Berlin, Germany, June 1998.
5. "Formation and Relaxation of 2D Island Distributions in Metal Epitaxy", 19th International Seminar on Surface Physics, Polanica Zdroj, Poland, June 1998.
6. "Growth and Relaxation of Metal Epitaxial Films: Ag/Ag(100)", Abteilung Theorie, Fritz-Haber-Institute, Berlin, Germany, June 1998.
7. "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:**

1. "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.
2. "Chemical Diffusion and Wave Propagation in Catalytic Surface Reactions", Joint US-Argentina Workshop on "Structure and Topography of Surfaces", La Plata, Argentina, November 1997.
3. "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.
4. "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.
5. "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.
6. "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.

**1996:**

1. "Growth and Equilibration of Metal(100) Homoepitaxial Films", Physics Department, University of Michigan, Ann Arbor, Michigan, September, 1996.
2. "Submonolayer Nucleation and Growth, and the Transition to Multilayer Kinetic Roughening during Metal(100) Homoepitaxy", NATO ASI on "Surface Diffusion", Rhodes, Greece, August, 1996.
3. "Growth and Equilibration of Metal Homoepitaxial Films", Institut de Physique Experimentale, EPF Lausanne, Lausanne, Switzerland, July, 1996.
4. "Non-linear Diffusion and Chemical Wave Propagation in Surface Reactions", CECAM Workshop on
5. "Pattern Formation in Surface Reactions", Lyon, France, June, 1996.
6. "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:**

1. "Modeling of Wave Propagation and Explosions in Surface Reactions", European Science Fdn. Workshop: "Adsorption & Catalytic Reaction Dynamics at Surfaces", Monterosso, Italy, Dec., 1995.
2. "Transition to Multilayer Kinetic Roughening", Gordon Research Conference on "Epitaxial Thin Films and Interfaces", New Hampshire, July 1995.
3. "From Submonolayer to Multilayer Growth in Metal (100) Homoepitaxy", Institut für Oberflächen Chemie, Universität, Ulm, Germany, May 1995.
4. "Diffraction Studies of Kinetically Roughening Epitaxial Films", Institut für Festkörperphysik, Universität, Hannover, Germany, May 1995.
5. "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.
6. "Epitaxial Thin Film Growth", Dept. of Physics, Univ. of Missouri at Columbia, March 1995.
7. "Nucleation, Growth, and Kinetic Roughening of Epitaxial Thin Films," WE-Hereaus Seminar on "Fundamentals of Epitaxial Growth," Physikzentrum Bad Honnef, Germany, February 1995.
8. "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:**

1. "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.
2. "Far-From-Equilibrium Surface Adsorption and Reaction Processes", Department of Chemistry and Laboratory for Surface Studies, University of Wisconsin-Milwaukee, October 1994.
3. "Nucleation, Growth, and Roughening of Thin Films," Plenary Lecture for Symposium on "Experiments and Simulations of Surface Processes", San Luis, Argentina, August 1994.
4. "Interface Propagation and Nucleation Phenomena for First-Order Poisoning Transitions," Symp. on "Phase Transitions in Catalytic Surface Reaction Models," IMA, U. Minnesota, June 1994.
5. "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.
6. "Hybrid Models for Spatiotemporal Behavior in Surface reactions", *ibid*, Cambridge, April 1994.
7. "A Lattice-Gas Model mimicking the NO + CO Reaction in Pt(100), *ibid*, Cambridge, April 1994.
8. "Far-From-Equilibrium Processes at Surfaces," Physics Dept., Georgia Tech., Atlanta, Feb. 1994.

**1993 AND EARLIER:**

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

3. "Nucleation and Growth in Metal-on-FCC(100) Metal Epitaxy," Abteilung für Oberflächenchemie and Katalyse, Universität Ulm, Ulm, Germany, June 1993.
4. "Simple Lattice-Gas Model for the NO + CO Reaction on Pt(100)," CECAM Workshop: Random Sequential Addition and Generalizations, Orsay-France, June 1993
5. "Spatial Correlations for Cooperative Sequential Adsorption with Clustering and Limiting Continuum Processes," *ibid*, Orsay, France, June 1993.
6. "Irreversible Island Formation during Deposition: Size & Separation Distributions; Diffraction Profiles," U.S.-Japan Seminar on Surface Characterization, Hawaii, March 1993.
7. "Scaling of Roughness & Bragg-Oscillation Decay during Low-Temp. Epitaxial Growth," *ibid* 1993.
8. "Modeling Surface Adsorption & Reaction Processes," Chemical Eng. Dept., Purdue, Jan. 1993.
9. "Spatio-Temporal Behavior in Surface Reactions: Mean-Field versus Lattice-Gas Modelling," Physics Department, Clarkson University, Potsdam, December 1992.
10. "Irreversible Island Formation in Surface Deposition Processes: Island Size and Separation Distributions," Institute für Festkörperphysik, Universität Hannover, Hannover, August 1992.
11. "Comparison of Mean-Field, Lattice-Gas, and Hybrid Models of Surface Reaction", Fritz-Haber-Institute der Max-Planck-Gesellschaft, Berlin, August, 1992.
12. "Far-From-Equilibrium Thin-Film Growth Processes," DRECAM/SRSIM Division; Commissariat a L'Energie Atomique Saclay, Gif-sur-Yvette, France, July 1992.
13. "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.
14. "Applic. of Random & Cooperative Sequential Adsorption to Chemisorption Processes," *ibid* 1992.
15. "Kinetic Phase Transitions in Surface Reactions," Dept. Chem. Eng., U. Minnesota, April 1992.
16. "Kinetic Phase Diagrams for Catalytic Surface Reactions," Department of Chemical Engineering, University of California, Santa Barbara, March 1992.
17. "Stochastic Models for Surface Adsorption," Dept. of Statistics, University of Iowa, November 1991.
18. "Modeling of Epitaxial Thin-Film Growth at Low-Temperature," Institute für Festkörperphysik, Universität Hannover, Hannover, August 1991.
19. "Bistability versus Discontinuous Transitions in Lattice Models of Catalytic Reactions," Fritz-Haber-Institute der Max-Planck-Gesellschaft, Berlin, August 1991.
20. "Modeling of Epitaxial Thin-Film Growth at Low-Temperature," Institute für Festkörperforschung, Forschungszentrum KFA, Jülich, July 1991.
21. "Kinetic Phase Transition, Catalytic Reactions, and Epidemics," Institute für Theoretische Physik der Universität zu Köln, Köln, July 1991.
22. "Characterization of Non-Equilibrium Micro-Structure," Dept. Physics U. Auckland, NZ Aug. 1988.
23. "Non-Hermitian Hamiltonians in Arrangement Channel QM," Dept. Chem., UBC, Feb. 1983.
24. "On the Solution to Faddeev's Equations in Differential Form, Workshop on Few Body Problems, Brown University, August 1979
25. "Truncation of BBGKY type hierarchies in kinetic theory", Dept Math. Physics, U Adelaide, 1978.

**APPENDIX: Contributed Talks (T) and Posters (P); Seminars at ISU (S) (total ~ 100)**

- (T) “Fe and Cu deposition onto and intercalation into MoS<sub>2</sub>”, Physical Electronics Conf., UW Lacrosse Aug. 2023
- (T) “Reshaping of Pd nanocubes and octahedra”, American Soc. Crystal Growth Meeting, on-line, July 2021.
- (T) Reshaping of truncated Pd nanocubes: Atomistic modeling + TEM, March APS Meeting 2021
- (T) “Multiscale modeling of the catalytic conversion of PNB to aldol in mesoporous silica: pore diameter dependence of yield” Fall ACS Meeting, San Diego 2019.
- (T) “Ab-initio thermodynamics and kinetics for nanoislands and nanopits on metal(100) surfaces” March APS Meeting New Orleans, 2017.
- (T) “Assembly and stability of metallic nanoclusters on metal(100) surfaces: Predictive modeling with ab-initio kinetics” PEC Meeting, U. Arkansas, Fayetteville, AK, June 2016.
- (T) “Ab-initio KMC modeling of self-assembly kinetics for bimetallic epi NC’s” AVS Int Symp Baltimore 2014
- (T) “Ab-initio KMC modeling of self-assembly kinetics for bimetallic epi NC’s” MRS Symp WW Boston 2013
- (T) “Multi-functionalization of nanoporous catalytic materials to enhance yield” MRS Symp. AA Boston 2013.
- (T) “Atomistic and CG modeling of film growth on quasicrystals” MRS Symp KK Boston 2012
- (P) “Atomistic modeling of Ru NC formation on graphene/Ru(0001): TDA vs. KDA” MRS Symp. S Boston 2012.
- (T) “Conversion reactions in surface-functionalized mesoporous silica...” MRS Symp. RR Boston 2011.
- (T) “Formation on Ni-rich nanostructures and adlayers on NiAl(110)...” MRS Symp. EE Boston 2011
- (T) “Morphological evolution during growth+erosion on Si(100): e-structure...to CG” MRS Symp EE Boston 2011
- (T) “Capture zone area distributions for homogeneous nucleation and growth of islands...” March APS Dallas 2011
- (S) “Stochastic models for spatial epidemics”, Computational Applied Math seminar, ISU Jan 2011
- (T) “Formation of irregular Al islands on NiAl(110)...” MRS Symp. UU Boston 2010
- (T) “Far-from equilibrium film growth on alloy surfaces: Ni and Al on NiAl(110)”, March APS Mtg, Portland 2010.
- (S) “Growth and relaxation in epitaxial thin films”, Physics Colloquium, ISU, February 2010.
- (T) “Atomistic and Coarse-Grained Continuum Modeling of Complex Physical Systems”, CAM ISU Math 2009.
- (S) “Far-From-Equilibrium Surface Reaction Processes”, Ames Lab, Chem. Physics review by ISU, April 2009.
- (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.
- (S) “Atomistic and Coarse-Grained Continuum Modeling of Reaction Processes”, CAM Seminar ISU Math, 2007.
- (S) “Realistic Modeling of Complex Physical and Chemical Systems”, Grad Student Colloq., ISU Math, Fall 2007.
- (S) “Far-From-Equilibrium Surface Reaction Processes”, Ames Lab, Chem Physics on-site review, April 2007.
- (S) “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.
- (S) “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”, 9<sup>th</sup> Int. QC Conf., ISU, Ames IA May 2005
- (P) “Atomistic & Continuum Modeling of Thin Film Growth”, IMA, U. Minn. MN, April 2005



- (S) "Growth & Equilibration of Epitaxial Metal Films: Modeling & Expt", ISU MSE Dept Colloqu..., March 2005.
- (S) "Atomistic and Continuum Modeling of Epitaxial Thin Film Growth", CAM Seminar, ISU Math Dept. Jan 2005
- (S) "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.
- (S) "Far-From-Equilibrium Surface Reaction Processes", Ames Lab, Chem Physics on-site review, April 2004.
- (S) "KMC, Hybrid, Multiscale Simulation Approaches to Surface...", Ames Lab Sci-DAC Review, Apr 2004
- (T) "Geometry-based Simulation of Submonolayer Film Growth" 50<sup>th</sup> AVS, Baltimore, MD Nov. 2003
- (S) "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.
- (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.
- (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)", 44<sup>th</sup> 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 Conf. Catalysis/Surface Chem, Texas, May, 1996.
- (S) "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
- (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 1<sup>st</sup> 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 1<sup>st</sup> 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.
- (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," 15<sup>th</sup> 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," 14<sup>th</sup> Midwest Theo Chem Conf., U. Chicago, May 1981.
- (P) "Exact Solution for some IVP's in Kinetic Theory," 14<sup>th</sup> 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.