

Charles Bruce Musgrave

Robert H. Davis Professor of Chemical and Biochemical Engineering
Associate Dean for Graduate Education, College of Engineering and Applied Science
University of Colorado at Boulder

EDUCATION

- Ph.D. Materials Science
 California Institute of Technology, Pasadena, California
 September 1994
 Advisor: William A. Goddard, III
- M.S. Materials Science
 California Institute of Technology, Pasadena, California
 May 1990
- B.S. Materials Science and Engineering
 University of California, Berkeley, California
 May 1988

EMPLOYMENT EXPERIENCE

- 2020 – Associate Dean for Graduate Education, College of Engineering and Applied
 Science
 University of Colorado Boulder, Boulder, CO
- 2016 – 2020 Chair, Department of Chemical and Biological Engineering
 University of Colorado Boulder, Boulder, CO
- 2016 – 2021 Joint Appointment, National Renewable Energy Laboratory
 Department of Energy, Golden, CO
- 2012 – Professor of Chemical and Biological Engineering
 University of Colorado Boulder, Boulder, CO
- 2012 – Fellow, Materials Science and Engineering Program
 University of Colorado Boulder, Boulder, CO
- 2011 – 2016 Associate Chair and Director of the Graduate Program of the Department of
 Chemical and Biological Engineering
 University of Colorado Boulder, Boulder, CO
- 2011 – Professor by Courtesy of Chemistry and Biochemistry
 University of Colorado Boulder, Boulder, CO
- 2011 – Fellow, Renewable and Sustainable Energy Institute
 University of Colorado Boulder, Boulder, CO
- 2008 – 2012 Associate Professor of Chemical and Biological Engineering
 University of Colorado Boulder, Boulder, CO
- 2004 – 2008 Assistant Professor of Chemical Engineering
 Stanford University, Stanford, CA
- 2003 – 2004 Visiting Professor of Chemistry and Chemical Biology
 Harvard University, Cambridge, MA

- 1996 – 2004 Assistant Professor of Chemical Engineering and Materials Science and Engineering
Stanford University, Stanford, CA
- 1995 – 1996 Postdoctoral Research Scientist, Department of Chemical Engineering
Massachusetts Institute of Technology, Cambridge, MA
Advisor: Klavs F. Jensen
- 1994 – 1995 Postdoctoral Research Scientist, Department of Chemistry
California Institute of Technology, Pasadena, CA
Advisor: William A. Goddard III

AWARDS AND HONORS

- 2020 Boulder Faculty Assembly Award for Excellence in Research, Scholarship and Creative Work, University of Colorado Boulder
- 2017 Outstanding Research Award, College of Engineering, University of Colorado Boulder
- 2017 Outstanding Service Award, Department of Chemical and Biological Engineering, University of Colorado Boulder
- 2013 Undergraduate Teaching Award, Department of Chemical and Biological Engineering, University of Colorado Boulder
- 2003 NSF US-Japan Nanoscience and Technology Young Scientist Exchange Program
- 2003 AIChE NorCal Excellence Award for Academic Teaching
- 1997 Charles Powell Fellow, Stanford University
- 1993 First Feynman Prize in Nanotechnology
- 1989 National Science Foundation Minority Fellowship (Declined)
- 1989 Ford Foundation Fellowship (Declined)
- 1989 National Defense Science and Engineering Grant Fellowship
- 1988 Graduate Degrees for Minorities in Engineering and Science (GEM) Fellowship
- 1986 Douglas G. Allen Scholarship, University of California, Berkeley
- 1986 Tau Beta Pi-Engineering Honor Society
- 1985 Ida Sproul Scholarship, University of California, Berkeley
- 1984 National Hispanic Scholars Scholarship

PROFESSIONAL ACTIVITIES

Affiliations

Fellow of the Materials Science and Engineering Program, University of Colorado at Boulder, September 2012 –

Fellow of the Renewable and Sustainable Energy Institute of the University of Colorado at Boulder and National Renewable Energy Laboratory, January 2011 -

Affiliate of the Renewable and Sustainable Energy Institute of the University of Colorado at Boulder and National Renewable Energy Laboratory, January 2009 - January 2011

Affiliate of the Woods Institute for the Environment, Stanford University, 2004-2008

Society Memberships

American Chemical Society

American Institute of Chemical Engineers
American Institute of Physics
American Physical Society
American Vacuum Society
Electrochemical Society
Materials Research Society

Reviewerships (partial list)

ACS Materials and Interfaces
Advanced Functional Materials
Advanced Energy Materials
Applied Physics Letters
Chemical Physics Letters
Chemistry of Materials
IEEE Transactions on Nanotechnology
Inorganic Chemistry
Journal of Applied Physics
Journal of Chemical Physics
Journal of Physical Chemistry
Journal of the American Chemical Society
Journal of Crystal Growth
Journal of the Electrochemical Society
Journal of Molecular Catalysis
Langmuir
Nanoletters
Nanotechnology
Nature Chemistry
Nature Communications
Physical Review B
Science
Science Advances
Surface Science
Surface Science Letters
Thin Solid Films

Internal Service Activities-Stanford

Co-chair of the Materials Initiative Computational Materials Science Laboratory
Chair of the Chemical Engineering Undergraduate Program, 2002-2007.
School of Engineering Computational Science Committee, (2005).
Latino-Chicano Faculty Committee
Faculty Search Committees in Chemical Engineering and Materials Science and Engineering.
Chemical Engineering Graduate Program Review, 2004-2005.
Chemical Engineering Undergraduate Program Review, 2005-2007.
Chemical Engineering Minority Student Advisor, 2000-2007.
Faculty Representative for Department Computing Systems, 1999-2007.
Department Website Developer and Webmaster, 1997-2003

Faculty Advisor to the American Institute of Chemical Engineers Student Chapter, 2003.
Graduate Admissions Committee – Department of Chemical Engineering, 2001-2005.
School of Engineering Courselet Program – Quantum Simulations
Stanford Engineering and Science Institute Short Course – ALD of High-κ Materials, 2004.

Internal Service Activities-University of Colorado

Chair – Department Improvement Committee, 2008-2011.
Organized Department Retreats, 2009, 2010.
Organized Department Advisory Board, 2009, 2010.
Chair-Department Strategic Plan Committee, 2009-2010.
Department Strategic Plan Committee, 2010-2011
Co-chair Department Graduate Admissions, 2009-2010
Faculty Mentor – Prof. Arthi Jayaraman, 2008-2014
Department Fundraising and Alumni Relations Committee, 2011
Biotechnology Building Design Committee - Computer Server Room
East Campus Master Plan Vision Subcommittee, 2010-2011
Boulder Campus Cyberinfrastructure Board, 2011-2016
Faculty Search Committees, Department of Chemical and Biological Engineering
Chair Search Committee, Department of Chemical and Biological Engineering 2012
Campus Representative - Colorado Collaborative Research Computing Board, 2011- 2016
Chair - Curriculum Development Committee - Materials Science Program, 2011- 2012
University Executive Advisory Council to the Graduate School, 2011- 2013
Associate Chair, Graduate Program Director, Department of Chemical and Biological Engineering, 2011- 2016
Executive Committee - Materials Science Program, 2012 - 2016
Graduate Admissions Committee - Materials Science Program, 2013 -
FLAG Leadership Committee, College of Engineering 2013 - 2014
Strategic Hiring Committee, RASEI, 2014 - 2016
Faculty Affairs Professional Development Director Search Committee, 2018
Engineering Dean Search Committee, College of Engineering and Applied Sciences, 2019-2020
Social Distancing Implementation Committee, College of Engineering and Applied Science - 2020
Department Chair, Department of Chemical and Biological Engineering, 2016 - 2020
Associate Dean for Graduate Education, College of Engineering and Applied Science, 2020 -
First Level Review Committee, College of Engineering and Applied Science, 2020 - 2023
Graduate Program Committee, Materials Science and Engineering Program, 2020 -
Graduate Program Committee, Department of Chemical and Biological Engineering, 2020 -
Graduate Mentoring Committee, Graduate School, 2022 -
CUBit Quantum Initiative, Education Committee, University of Colorado Boulder, 2023 -

External Service Activities

AIChE Area 8 (Electronic Materials) Executive Committee
Northern California Chapter of the AIChE Professional Progress Award Committee
Feynman Prize in Nanotechnology Selection Committee
SRC Multi-scale and Multi-phenomena Modeling and Simulation Work Group
AVS Thin Film Users Group Executive Committee

Ph.D. Thesis Committee, Guanhua Chen, Department of Physics, Hong Kong University of Science and Technology, Hong Kong, China (2004)
Ph.D. Thesis Committee, Guillaume Mazaleyrat, Laboratoire d'Analyse et d'Architecture des Systèmes du CNRS, Université Paul Sabatier Toulouse III, Toulouse, France (2006)
Ph.D. Thesis Committee, Philippe de Rouffignac, Department of Chemistry, Harvard University, Cambridge, MA (2006)
Ph.D. Thesis Committee, Lars Nielsen, Department of Chemistry, Harvard University, Cambridge, MA (2006)
National Science Foundation, Multiple Panel Reviews.
Science Foundation Ireland, Nanoscience Research Center Review, Panel Chair, December 2012-January 2013.
King Abdullah University of Science and Technology Competitive Grants Program Review Panel (2018-)
Sustainability Advisory Board, City of Longmont, Colorado (2020-)
King Abdullah University of Science and Technology Postdoctoral Fellowship Review Committee (2022-)
119 Transportation Corridor Community Advisory Board, Boulder County, Colorado (2021-)

External Professional Activities

Advisor to Intel Corporation
Advisor to Applied Materials Corporation
Advisor/Consultant to Acorn Technologies
Advisor to and collaboration with Agilent Corporation
Advisor to Samsung Corporation
Advisor to Novellus Corporation
Advisor to Torrex Corporation (acquired by Applied Materials 2004)
Advisor to LSI Logic Corporation
Consultant for SC Solutions Corporation
Advisor to Motorola Corporation
Advisor to KLA-Tencor Corporation
Collaboration with General Motors Corporation
Collaboration with Xerox Corporation
Consultant to Vulcan Incorporated
Advisor to Khosla Ventures
Advisor to Zyvex Corporation
Advisor to Lux Capital
Advisor to First Green Partners

CONFERENCE PROGRAM CHAIRS AND ORGANIZING COMMITTEES

Co-Organizer, *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the American Vacuum Society*, Stanford University, June 27, 2002.
Program Review Committee, 29th International Symposium on Combustion, Combustion Institute, Tokyo, Japan, July 2003.
Organizing Committee, *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the American Vacuum Society*, University of California, Berkeley, June 11, 2003.

Program Vice-Chairman, Area 8e, Electronic and Photonic Materials, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

Electronic Materials Topical Conference Vice-Chair, Materials for Microelectronics, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

Program Review Committee, 30th International Symposium on Combustion, Combustion Institute, Chicago, IL, July 2004.

Program Chair, Area 8e, Electronic and Photonic Materials, *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.

Organizing Committee, *American Vacuum Society Atomic Layer Deposition 2005 Conference*, San Jose, CA, August 2005.

Organizing Committee, *Renewable Energy Topical Conference, American Vacuum Society International Symposium*, Boston, MA, October 2005.

Organizing Committee, *American Vacuum Society Atomic Layer Deposition 2006 Conference*, Seoul, Korea, August 2006.

Program Chair, Area 8e, Electronic and Photonic Materials, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.

Organizing Committee, *North American Catalysis Society National Meeting*, Denver, CO, 2017

Electronic Materials Topical Conference co-Chair, Materials for Microelectronics, *American Institute of Chemical Engineers Annual Meeting*, Boston, MA, November 2021.

CONFERENCE SESSION CHAIRS

Session Vice-Chair, Fundamentals of Surface Processes on Semiconductors, *American Institute of Chemical Engineers Annual Meeting*, Miami, FL, November 1998.

Session Chair, Semiconductor Surface Chemistry: Reactions Involving Metals, *American Chemical Society National Meeting*, San Francisco, CA, March 2000.

Session Chair, Semiconductor Surface Chemistry, *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.

Session Co-Chair, Reaction Kinetics in Electronic Materials Processing, *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

Session Chair, Nanoparticle Coatings and Molecular Simulation of Materials Processes, *American Institute of Chemical Engineers Annual Meeting*, Indianapolis, IN, November 2002.

Session Chair, High-K Dielectrics, *The Third American Vacuum Society Topical Conference on Atomic Layer Deposition*, San Jose, CA, August 2003.

Session Chair, Semiconductor Surface Chemistry, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

Plenary Session Vice-Chair, Advanced Microelectronic Processing, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

Session Chair, Chemical Vapor Deposition of Electronic Materials, *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.

Session Vice-Chair, Reaction Kinetics in Electronic Materials Processing, *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.

Session Chair, Atomic Layer Deposition of Electronic Materials, *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.

Session Chair, Atomic Layer Deposition, *American Institute of Chemical Engineers Annual Meeting*, Cincinnati, OH, November 2005.

Session Chair, Fabrication and Assembly of 1-D Nanostructures, *American Institute of Chemical Engineers Annual Meeting*, Cincinnati, OH, November 2005.

Session Co-chair, Surface Reaction Kinetics in Semiconductor Processing, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.

Session Chair, Modeling and Simulation of Organic Semiconductor Systems, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.

Session Chair, Complex and Crystalline Oxides, *Materials Research Society Spring Meeting*, San Francisco, CA, April 2007.

Session Chair, Atomic Layer Deposition, *American Institute of Chemical Engineers Annual Meeting*, Salt Lake City, UT, November 2007.

Session Chair, Atomic Layer Deposition, *American Institute of Chemical Engineers Annual Meeting*, Philadelphia, PA, November 2008.

Session Chair, Organic Photovoltaics, *Inter-Continental Advanced Materials for Photonics Summer School*, Boulder, CO, July 2012.

Session Chair, Catalysis Modeling and Simulation, *North American Catalysis Society Meeting*, Denver, CO June 2017.

Session Chair, Advanced Batteries, *American Institute of Chemical Engineers Meeting*, Boston, MA November 2021.

PUBLICATIONS

ARTICLES IN REFEREED JOURNALS

1. Musgrave, C., J. Perry, R. Merkle and W. Goddard III, "Theoretical Studies of a Hydrogen Abstraction Tool for Nanotechnology," *Nanotechnology* 2, 187-195 (1991).
2. Musgrave, C., S. Dasgupta and W. Goddard III, "Hessian Biased Force Field for Polysilane Polymers," *Journal of Physical Chemistry* 99, 13321-13333 (1995). DOI: 10.1021/j100036a004
3. Musgrave, C., S. Harris and W. Goddard III, "The Surface-Radical-Surface-Olefin Recombination Step for CVD Growth of Diamond. Calculation of the Rate Constant from

- First Principles,” *Chemical Physics Letters* 247, 359-365 (1995). DOI: 10.1016/S0009-2614(95)01243-5
4. Ricca, A., C. Bauschlicher, J. Kang and C. Musgrave, “H Abstraction from a Diamond (111) Surface in a Uniform Electric Field,” *Surface Science* 429, 199-205 (1999). DOI: 10.1016/S0039-6028(99)00377-5
 5. Ricca, A. and C. Musgrave, “Theoretical Study of the Cl-Passivated Si (111) Surface,” *Surface Science* 430, 116-125 (1999). DOI: 10.1016/S0039-6028(99)00407-0
 6. Wang, G., C. Mui, C. Musgrave and S. Bent, “Cycloaddition of Cyclopentadiene and Dicyclopentadiene on Si (100)-2×1: Comparison of Monomer and Dimer Adsorption,” *Journal of Physical Chemistry B* 102, 6803-6808 (1999). DOI: 10.1021/jp991528x
 7. Widjaja, Y., M. Mysinger and C. Musgrave, “An Ab Initio Study of Adsorption and Decomposition of NH₃ on Si (100)-2×1,” *Journal of Physical Chemistry B* 104, 2527-2533 (2000). DOI: 10.1021/jp9936998
 8. Mui, C., S. Bent and C. Musgrave, “A Theoretical Study of the Structure and Thermochemistry of 1,3-butadiene on the Ge/Si (100)-2×1 Surface,” *Journal of Physical Chemistry A* 104, 2457-2462 (2000). DOI: 10.1021/jp991797n
 9. Kang, J. and C. Musgrave, “A Theoretical Study of the Chemical Vapor Deposition of (100) Diamond: An Explanation for the Slow Growth of the (100) Surface,” *Journal of Chemical Physics* 113, 7582 (2000). DOI: 10.1063/1.1311976
 10. Widjaja, Y. and C. Musgrave, “A DFT Study of Nonlocal Effects on NH₃ Adsorption and Dissociation on Si (100)-2×1,” *Surface Science* 469, 9-20 (2000). DOI: 10.1016/S0039-6028(00)00810-4
 11. Senosiain, J., J. Han, C. Musgrave, and D. Golden, “Use of Quantum Methods for a Consistent Approach to Combustion Modeling: Hydrocarbon Bond Dissociation Energies,” *Faraday Discussions* 119 (2001). DOI: 10.1039/B103011F
 12. Senosiain, J., C. Musgrave, and D. Golden, “Use of Quantum Methods with Transition State Theory; Application to the H-Atom Metathesis Reactions,” *Journal Physical Chemistry A* 105, 1669-1675 (2001). DOI: 10.1021/jp002424l
 13. Wang, G., C. Mui, C. Musgrave, and S. Bent, “Effect of a Methyl-Protecting Group on the Adsorption of Pyrrolidine on Si (100)-2×1,” *Journal Physical Chemistry B* 105, 3295-3299 (2001). DOI: 10.1021/jp004298r
 14. Mui, C., G. Wang, S. Bent, and C. Musgrave, “Reactions of Methylamines at the Si(100)-2×1 Surface,” *Journal of Chemical Physics* 114, 10170-10180 (2001). DOI: 10.1063/1.1370056
 15. Kang, J. and C. Musgrave, “The Effect of an STM Electric Field on the Chemical Vapor Deposition of (100) Diamond,” *Nanotechnology* 12, 258 (2001).
 16. Widjaja, Y., and C. Musgrave, “An Ab Initio Study of the Initial Growth Mechanism of Silicon Nitride on Si (100)-2×1 Using NH₃,” *Physical Review B* 64, 205303-205312 (2001). DOI: 10.1021/jp9936998

17. Hall, M., C. Mui, and C. Musgrave, "DFT Study of the Adsorption of Chlorosilanes on the Si (100) Surface," *Journal of Physical Chemistry B* 105, 12068-12075 (2001). DOI: 10.1021/jp0118874
18. Kang, J. and C. Musgrave, "A Theoretical Study of the Chemical Vapor Deposition of (100) Silicon from Silane," *Physical Review B* 64, 245330-245340 (2001). DOI: 10.1103/PhysRevB.64.245330
19. Wang, G., C. Mui, C. Musgrave, and S. Bent, "Example of a Thermodynamically Controlled Reaction on a Semiconductor Surface: Acetone on Ge (100)-2 \times 1," *Journal of Physical Chemistry B* 105, 12559-12565 (2001). DOI: 10.1021/jp013058o
20. Lee, S., C. Musgrave, P. Zhao, and J. Stebbins, "Topological Disorder and Reactivity of Borosilicate Glasses: Quantum Chemical Calculations and ^{12}O and ^{11}B NMR Study," *Journal of Physical Chemistry B* 105, 12583-12595 (2001). DOI: 10.1021/jp012119f
21. Kang, J. and C. Musgrave, "Prediction of Transition State Barriers and Enthalpies of Reaction by a New Hybrid Density-Functional Approximation," *Journal of Chemical Physics* 115, 11040-11051 (2001). DOI: 10.1063/1.1415079
22. Kang, J. and C. Musgrave, "The Mechanism of HF/H $_2$ O Chemical Etching of SiO $_2$," *Journal of Chemical Physics* 116, 275-280 (2002). DOI: 10.1063/1.1420729
23. Kang, J. and C. Musgrave, "The Mechanism of Atomic Layer Deposition of SiO $_2$ on the Silicon (100)-2 \times 1 Surface Using SiCl $_4$ and H $_2$ O as Precursors," *Journal of Applied Physics* 91, 3408-3414 (2002). DOI: 10.1063/1.1436294
24. Widjaja, Y. and C. Musgrave, "A DFT Study of Atomic Nitrogen on the Si(100)-(2 \times 1) Surface," *Journal Physical Chemistry B* 106, 2643-2648 (2002). DOI: 10.1021/jp013335r
25. Widjaja, Y. and C. Musgrave, "Atomistic Mechanism of the Initial Oxidation of the Clean Si (100)-2 \times 1 Surface by O $_2$ and SiO $_2$ Decomposition," *Journal of Chemical Physics* 116, 5774-5780 (2002). DOI: 10.1063/1.1456036
26. Mui, C., J. Han, G. Wang, C. Musgrave, and S. Bent, "Proton Transfer Reactions on Semiconductor Surfaces," *Journal of the American Chemical Society* 124, 4027-4038 (2002). DOI: 10.1021/ja0171512
27. Widjaja, Y. and C. Musgrave, "Quantum Chemical Study of the Mechanism of Aluminum Oxide Atomic Layer Deposition," *Applied Physics Letters* 80, 3304-3306 (2002). DOI: 10.1063/1.1473237
28. Kang, J. and C. Musgrave, "A Quantum Chemical Study of the Self-Directed Growth Mechanism of Styrene and Propylene Molecular Nanowires on the Silicon (100) 2 \times 1 Surface," *Journal of Chemical Physics* 116, 9907-9913 (2002). DOI: 10.1063/1.1476005
29. Widjaja, Y. and C. Musgrave, "Quantum Chemical Study of the Elementary Reactions in Zirconium Oxide Atomic Layer Deposition," *Applied Physics Letters* 81, 304-306 (2002). DOI: 10.1063/1.1490415
30. Wang, G., C. Mui, C. Musgrave, and S. Bent, "Competition and Selectivity of Organic Reactions on Semiconductor Surfaces: Reaction of Unsaturated Ketones on Si (100)-2 \times 1 and Ge (100)-2 \times 1," *Journal of the American Chemical Society* 124, 8990-9904 (2002). DOI: 10.1021/ja026330w

31. Widjaja, Y. and C. Musgrave, "Atomic Layer Deposition of Hafnium Oxide: A Detailed Reaction Mechanism from First Principles," *Journal of Chemical Physics* 117, 1931-1934 (2002). DOI: 10.1063/1.1495847
32. Filler, M., C. Mui, G. Wang, C. Musgrave, and S. Bent, "Competition and Selectivity in the Reaction of Nitriles on Ge (100)-2×1," *Journal of the American Chemical Society* 125, 4928-4936 (2003). DOI: 10.1021/ja027887e
33. Wang, G., C. Mui, J. Tannaci, M. Filler, C. Musgrave and S. Bent; "Reactions of Cyclic Aliphatic and Aromatic Amines on Ge (100)-2x1 and Si (100)-2×1," *Journal of Physical Chemistry B* 107, 4983-4996 (2003). DOI: 10.1021/jp026864j
34. Song, S., D. Golden, R. Hansen, C. Bowman, J. Senosiain, C. Musgrave, and G. Friedrichs, "A Shock Tube Study of the Reaction $\text{NH}_2 + \text{CH}_4 \rightarrow \text{NH}_3 + \text{CH}_3$ and Comparison with Transition State Theory," *International Journal of Chemical Kinetics* 35, 304-309 (2003). DOI: 10.1002/kin.10131
35. Akis, R., D. Ferry, C. Musgrave, "Kinetic Lattice Monte Carlo Simulations of Processes on the Silicon (100) Surface," *Physica E-Low Dimensional Systems and Nanostructures* 19, 183-187 (2003). DOI: 10.1016/S1386-9477(03)00331-X
36. Senosiain, J., C. Musgrave and D. Golden, "Temperature and Pressure Dependence of the Reaction of OH and CO: Master Equation Modeling on a High-Level Potential Energy Surface," *International Journal of Chemical Kinetics* 35, 464-474 (2003). DOI: 10.1002/kin.10144
37. Widjaja, Y., J. Han and C. Musgrave, "Quantum Chemical Study of Zirconium Oxide Deposition on the Si (100)-2×1 Surface," *Journal of Physical Chemistry B* 107, 9319-9324 (2003). DOI: 10.1021/jp030257u
38. Mui, C., M. Filler, S. Bent, and C. Musgrave, "Reactions of Nitriles at Semiconductor Surfaces," *Journal of Physical Chemistry B* 107, 12256-12267 (2003). DOI: 10.1021/jp034864t
39. Widjaja, Y. and C. Musgrave, "Indirect Adsorbate-Adsorbate Interactions Mediated Through the Surface Electronic Structure of the Si (100)-(2×1) Surface," *Journal of Chemical Physics* 120, 1555-1559 (2004). DOI: 10.1063/1.1631932
40. Han, J., G. Gao, Y. Widjaja, E. Garfunkel, and C. Musgrave, "A Quantum Chemical Study of ZrO_2 Atomic Layer Deposition Growth Reactions on the SiO_2 Surface," *Surface Science* 550, 199-212 (2004). DOI: 10.1016/j.susc.2003.12.030
41. Xu, Y. and C. Musgrave, "A DFT Study of the Al_2O_3 Atomic Layer Deposition on SAMs: Effect of SAM Termination," *Chemistry of Materials*, 16, 646-653 (2004). DOI: 10.1021/cm035009p
42. Pomerantz, A., J. Han, and C. Musgrave, "Calculating Cumulene/Poly-yne Isomerization Energies," *Journal of Physical Chemistry A*, 108, 4030-4035 (2004). DOI: 10.1021/jp0372744
43. Heyman, A. and C. Musgrave, "A Quantum Chemical Study of Atomic Layer Deposition of Al_2O_3 Using AlCl_3 and H_2O as Precursors," *Journal of Physical Chemistry B*, 108, 5718-5725 (2004). DOI: 10.1021/jp049762x

44. Mui, C., Y. Widjaja, J. Kang, and C. Musgrave, "Surface Reaction Mechanisms for Atomic Layer Deposition of Silicon Nitride," *Surface Science*, 557, 159-170, (2004). DOI: 10.1016/j.susc.2004.03.029
45. Mui, C., S. Bent and C. Musgrave, "A Density Functional Theory Study on the Effect of Ge Alloying on Hydrogen Desorption from SiGe Alloy Surfaces," *Journal of Physical Chemistry B*, 108, 6336-6350 (2004). DOI: 10.1021/jp037948a
46. Mui, C. and C. Musgrave, "Atomic Layer Deposition of HfO₂ Using Alkoxides as Precursors," *Journal of Physical Chemistry B*, 108, 15150-15164 (2004). DOI: 10.1021/jp037507r
47. Mui, C., S. Bent and C. Musgrave, "A Quantum Chemistry Based Statistical Mechanical Model of Hydrogen Desorption from Si (100)-2×1, Ge(100)-2×1, and SiGe Alloy Surfaces," *Journal of Physical Chemistry B*, 108, 18243-18253, (2004). DOI: 10.1021/jp0379493
48. Mui, C. and C. Musgrave, "Initial Oxidation and Hydroxylation of the Ge (100)-2×1 Surface by Water and Hydrogen Peroxide," *Langmuir*, 20, 7604-7609 (2004). DOI: 10.1021/la0498410
49. Yoon, T., C. Musgrave, S. Johnson and G. Brown, Jr., "Adsorption of Organic Matter at Mineral/Water Interfaces: I. ATR-FTIR Spectroscopic and Quantum Chemical Study of Oxalate Adsorbed at the Boehmite (γ -AlOOH)/Water and Corundum (α -Al₂O₃)/Water Interfaces," *Geochimica et Cosmochimica Acta*, 68, 4505-4518 (2004). DOI: 10.1016/j.gca.2004.04.025
50. Centoni, S., B. Sadigh, G. Gilmer, T. de la Rubia and C. Musgrave, "First-Principles Calculation of Free Si (100) Surface Impurity Enrichment," *Applied Physics Letters*, 87, 232101-1-3 (2005). DOI: 10.1063/1.2138811
51. Huang, K., J. Han, A. Cole, C. Musgrave and R. Waymouth, "Homolysis of Weak Ti-O Bonds: Experimental and Theoretical Studies of Titanium Oxygen Bonds Derived from Stable Nitroxyl Radicals," *Journal of the American Chemical Society*, 127, 3807-3816 (2005). DOI: 10.1021/ja044512f
52. Centoni, S., B. Sadigh, G. Gilmer, T. Lenosky, T. de la Rubia and C. Musgrave, "First-Principles Calculation of Intrinsic Defect Formation Volumes in Silicon," *Physical Review B*, 72, 195206-1-9 (2005). DOI: 10.1103/PhysRevB.72.195206
53. Xu, Y. and C. Musgrave, "Atomic Layer Deposition of Hafnium Nitrides Using Ammonia and Alkylamide Precursors," *Chemical Physics Letters*, 407, 272-275 (2005). DOI: 10.1016/j.cplett.2005.03.084
54. Mui, C. and C. Musgrave, "Initial Nitridization of the Ge (100) 2×1 Surface by Ammonia," *Langmuir*, 21, 5230-5232 (2005). DOI: 10.1021/la0470840
55. Xu, Y. and C. Musgrave, "Atomic Layer Deposition of HfO₂ on Nitridized Si Surfaces," *Applied Physics Letters*, 86, 192110-192113 (2005). DOI: 10.1063/1.1922080
56. Xu, Y. and C. Musgrave, "A Chemical Mechanism for Nitrogen Incorporation into HfO₂ ALD Films Using Ammonia and Alkylamides as Precursors," *Surface Science*, 591, L280-L285 (2005). DOI: 10.1016/j.susc.2005.06.032

57. Kelly, M., J. Han, C. Musgrave and G. Parsons, "In-Situ Infrared Spectroscopy and Density Functional Theory Modeling of Hafnium Alkylamine Adsorption on Si-OH and Si-H Surfaces," *Chemistry of Materials*, 17, 5305-5314 (2005). DOI: 10.1021/cm051064h
58. Solares, S., S. Dasgupta, Y. Kim, C. Musgrave, P. Schultz, and W. Goddard, "Density Functional Theory Study of the Geometry, Energetics and Reconstruction Process of Si (111) Surfaces," *Langmuir*, 21, 12404-12414 (2005). DOI: 10.1021/la052029s
59. Pornprasertsuk, R., P. Ramanarayanan, C. Musgrave and F. Prinz, "Predicting Ionic Conductivity of Solid Oxide Fuel Cell Electrolytes from First Principles," *Journal of Applied Physics*, 98, 1-8 (2005). DOI: 10.1063/1.2135889
60. Mukhopadhyay, A. and C. Musgrave, "Non-Growth Ligand Exchange Reactions in Atomic Layer Deposition of HfO₂," *Chemical Physics Letters*, 421, 215-220 (2006). DOI: 10.1016/j.cplett.2006.01.057
61. Mukhopadhyay, A., J. Sanz and C. Musgrave, "First-Principles Calculations of Structural and Electronic Properties of Monoclinic Hafnia Surfaces," *Physical Review B*, 73, 115330-115337 (2006). DOI: 10.1103/PhysRevB.73.115330
62. Huang, K., J. Han, C. Musgrave, and R. Waymouth, "Density Functional Theory Calculations on Ti-TEMPO Complexes: Influence of Ancillary Ligation on the Strength of the Ti-O bond," *Organometallics*, 25, 3317-3323 (2006). DOI: 10.1021/om060148c
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46. Mukhopadhyay, A., Zhang, Z. and Musgrave, C., "Simulations of HfO₂ Interfaces with Ge and GaAs," *Fall Materials Research Society Meeting*, Boston, MA, December 2007.
47. Musgrave, C., "Theoretical and Spectroscopic Studies of the Organic Functionalization of Semiconductor Surfaces," *American Chemical Society National Meeting*, New Orleans, LA, April, 2008.
48. Paul, A., Zimmerman, P. and C. Musgrave, "A Quantum Chemical Study of Ammonia Borane Dehydrogenation by Organometallic Complexes," *Indian Association of Cultivation of Science*, Kolkata, India, January 2009.
49. Holder, A., and C. Musgrave, "Quantum Chemical Simulations of OH Rotors as Two-Level Systems in Atomic Layer Deposited Al₂O₃ Qubit Dielectrics," *Coherent Superconducting Qubit Meeting*, San Diego, CA, April, 2010.
50. Musgrave, C., "Quantum Simulations: Staying One Step Ahead of Chemical Intuition," *Symposium in Honor of Roy Gordon*, Harvard University, Cambridge, MA, May, 2010.
51. Musgrave, C., "Quantum Mechanical Simulations of Atomic Layer Deposition," Plenary Talk; *The American Vacuum Society 10th International Conference on Atomic Layer Deposition*, Seoul, South Korea, June 2010.
52. Ryland, S., A. Derk and C. Musgrave, "Atomic and Molecular Layer Deposition; Insights from Theory," *The American Vacuum Society International Meeting*, Albuquerque, NM, October 2010.
53. Musgrave, C., "Nanostructures for Energy Capture and Conversion", The Renewable and Sustainable Energy Institute Annual Meeting, University of Colorado, Boulder, CO April 2011.
54. Musgrave, C., A. Holder, P. Zimmerman and Z. Zhang, "Carrier Multiplication by Singlet Fission in Conjugated Molecular Organic Materials," Singlet Fission Workshop, Golden, CO, May 2011.

55. Musgrave, C., "Guiding Principles For The Catalytic Reduction Of CO₂ From Theory," American Chemical Society Fall National Meeting, Denver, CO, August 2011.
56. Musgrave, C., "Singlet Fission in Organic Photovoltaics," American Physical Society March National Meeting, Boston, MA, February 2012.
57. Musgrave, C., "Chemical Mechanisms of Atomic Layer Deposition from First Principles Calculations," American Chemical Society Spring National Meeting, San Diego, CA, March 2012.
58. Musgrave, C., C. Lim, A. Holder, C. Bowman, "Design and Implementation of Novel Photoinitiators," Industry University Collaborative Research Center, St. Paul, MN, April 2012.
59. Musgrave, C., and A. Holder, "Singlet Fission Through Multiexcitonic Dark States in Conjugated Molecular Organic Materials," Singlet Fission Workshop, Lyons, CO, June 2012.
60. Musgrave, C., "Photoexcitation: Exciting Molecules," *Inter-Continental Advanced Materials for Photonics Summer School*, Boulder, CO, July 2012.
61. Musgrave, C., "Excited States: How to Properly Describe Excited States," *Inter-Continental Advanced Materials for Photonics Summer School*, Boulder, CO, July 2012.
62. Musgrave, C., "Excited State Processes: Conical Intersections, Conversions, Couplings, Crossings, etc.," *Inter-Continental Advanced Materials for Photonics Summer School*, Boulder, CO, July 2012.
63. Musgrave, C., "Exciton Multiplication: The Mechanism of Singlet Fission in OPV," *Inter-Continental Advanced Materials for Photonics Summer School*, Boulder, CO, July 2012.
64. Lim, C., A. Holder and C. Musgrave, "*The Mechanism of Homogeneous Catalytic Reduction of CO₂ by Pyridine*", Centre Europeen de Cacul Atomique et Moleculaire CO₂ Workshop, University of Bremen, Bremen Germany, October 2012.
65. Musgrave, C., "Mechanism of Li-ion Transport and Capacity Fading in LiCoO₂ cathodes via HF attack and the protective role of an alumina coating," American Chemical Society Spring National Meeting, New Orleans, LA, April 2013.
66. Musgrave, C., "Quantum Chemical Simulations of Chemical Mechanisms for Atomic Layer Deposition," American Chemical Society Fall National Meeting, Indianapolis, IN, September 2013.
67. Lim, C.H., A.M. Holder, C.B. Musgrave and J.T. Hynes, "Reduction of CO₂ to Methanol by an Organic Hydride via Hydride Transfer/Proton Transfer (HTPT) Steps," PCET 2014: Second International Conference on Proton-Coupled Electron Transfer, Uppsala, Sweden, June 2014.
68. Deml, A. M., V. Stevanovic, R. O'Hayre and C. B. Musgrave, "First principles insights into redox processes in oxides: An investigation of oxygen vacancy formation energetics," 2014 Electrochemistry Workshop, Monterey Bay, CA, 8 July 2014.

69. Musgrave, C., C. Lim, A. Holder, and J. Hynes, "Role of Pyridine as a Biomimetic Organo-hydride for Homogeneous Reduction of CO₂ to Methanol," American Chemical Society Fall National Meeting, San Francisco, August 2014.
70. Muhich, C.L., A.W. Weimer and C.B. Musgrave, "Rapid Computational Screening and Prototyping of Solar Thermal Water Splitting Materials," *Department of Energy Fuel Cells Technology Office*, Webinar, December 2014.
71. Musgrave, C.B., C.L. Lim, Y.C. Kuo, A.M. Holder, and J.T. Hynes, "Reduction of CO₂ to Methanol Catalyzed by Biomimetic Organo Hydrides," AFOSR CO₂ MURI Review, Invited External Speaker, San Diego, January 2015.
72. Lim, C.L., Y.C. Kuo, A.M. Holder, C.B. Musgrave, and J.T. Hynes, "Catalytic Mechanisms for Reducing CO₂ by Organo Hydride Catalysts," Third Biennial CO₂ Workshop, Princeton University, Princeton, N.J., March 2015.
73. Hynes, J.T., C.B. Musgrave, C.L. Lim, and A.M. Holder, "Reduction of CO₂ to methanol by an organic hydride via hydride transfer/proton transfer steps," *American Chemical Society Spring National Meeting*, Denver, March 2015.
74. Muhich, C., B. Ehrhardt, I. Al Shankiti, B. Ward, C. Musgrave and A. Weimer, "Needed Research Focus for Achieving Cost-Effective and Reliable Solar-Thermal Water Splitting," *The 227th Electrochemical Society Meeting*, Chicago, May 2015.
75. Muhich, C., B. Ehrhardt, I. Al Shankiti, B. Ward, C. Musgrave and A. Weimer, "Near-Isothermal Doped-hercynite Redox Cycle for Solar-thermal Water Splitting," *The 227th Electrochemical Society Meeting*, Chicago, May 2015.
76. Musgrave, C., C. Lim, and A. Holder, Hynes, J., and Y. Kuo, "Experimental and theoretical examination of the catalytic reduction of CO₂ by renewable organo hydrides based on heterocyclic aromatic amines," *American Chemical Society Fall National Meeting*, Boston, August 2015.
77. Weimer, A., V. Aston, C. Muhich, and C. Musgrave "Hybrid chemical looping hydrogen process using mixed metal oxides," *American Chemical Society Fall National Meeting*, Boston, August 2015.
78. Musgrave, C., C. Lim, Tong, C. Bowman "Ab Initio Design of Novel Polymerization Photoinitiators," Polymerization Fundamentals Meeting, Boulder, CO September 2015.
79. Musgrave, C., C. Lim, and A. Holder, Hynes, J., "The Catalytic Reduction of CO₂ by Renewable Organo Hydrides Based on Heterocyclic Aromatic Amines," *American Chemical Society Spring National Meeting*, San Diego, April 2016.
80. Lim, C., J. Theriot, G. Miyake and C. Musgrave, "Ab Initio Design of Organic Catalysts And Photocatalysts," American Chemical Society Spring National Meeting, San Diego, CA, March, 2016.
81. Young, M., A. Holder, S. George, and C. Musgrave "Band-Diagram Framework for Materials Development in Cation Intercalation Charge Storage," *American Chemical Society Spring National Meeting*, San Francisco, CA, April, 2017.
82. Trottier, R., S. Miller, C. Bartel, A. Holder, A. Weimer and C. Musgrave, "Rapid Computational Screening of Materials for Water Splitting Using Ab Initio and Machine

- Learned Models: Thermodynamic and Kinetics of Solar Thermal H₂ Generation,” *The 231st Electrochemical Society Meeting*, New Orleans, May 2017.
83. Young, M., A. Holder, C. Musgrave, “Unified Band Diagram Framework for the Development of Cation Intercalation Materials for Next Generation Batteries,” *The 231st Electrochemical Society Meeting*, New Orleans, May 2017.
 84. Millican, S., R. Trottier, C. Bartel, A.W. Weimer and C.B. Musgrave, “Incorporating Spin Disorder, Phase and High Temperature Free Energy into Rapid Computational Screening of Redox Materials for Water Splitting,” Invited Keynote Talk, *The 21st International Conference in Solid State Ionics*, Padova, Italy, June 2017.
 85. Musgrave, C., and C-H. Lim “Quantum Chemical Design of Organic Catalysts and Photocatalyst,” *Telluride Solar Solutions Workshop*, Telluride, CO, June 2017.
 86. Musgrave, C., S. Millican, Ryan Trottier, Aaron Holder and C. Bartell, “Ab Initio and Machine Learned Modeling and Design of New Materials,” *Telluride Workshop on Computational Materials Chemistry*, Telluride, CO, August 2017.
 87. Hynes, J, C. Lim, A. Holder and C. Musgrave, “Reduction of CO₂ to Methanol by an Organic Hydride via Hydride Transfer/Proton Transfer (HTPT) Steps,” *Japanese Society of Molecular Science*, Sendai, Japan, September 2017.
 88. Musgrave, C., C. Bartel, S. Miller and A. Holder, “A Machined Learned Model for the Prediction of the Free Energies of Materials and its Applications to Chemical Reactions involving Solids,” *American Chemical Society Spring National Meeting*, New Orleans, LA, April 2018.
 89. Musgrave, C., C. Bartel, C. Sutton, B. Goldsmith, A. Holder, “Discovery of New Halide Double Perovskite Photovoltaic Materials Using Machine Learning and Electronic Structure Theory,” *American Chemical Society Spring National Meeting*, Orlando, FL, March, 2019.
 90. Musgrave, C., A. Holder, and M. Young, “Unified Electrochemical Band Diagram Framework: Understanding the Driving Forces of Material Electrochemistry,” *American Chemical Society Spring National Meeting*, Orlando, FL, April 2019.
 91. Musgrave, C., S. Millican, Ryan Trottier, Aaron Holder and C. Bartel, “Ab Initio and Machine Learned Modeling, Design and Discovery of Water Splitting Materials,” *Materials Research Society Spring National Meeting*, Phoenix, AZ, March 2019.
 92. Musgrave, C., S. Millican, and Aaron Holder, “Combined Ab Initio and Machine Learning Approaches to Discover Materials for Hydrogen Generation,” *The 236th Electrochemical Society Meeting*, Atlanta, GA, October 2019.
 93. Musgrave, C., A. Alherz, N. Singstock, Y. Alsunni, P. Brimley, T. Whittaker, “Accurate Modeling of Electrochemical Reactions Using Grand Canonical Density Functional Theory,” *American Chemical Society National Meeting*, San Diego, CA, March 2022.
 94. Musgrave, C., N. Singstock, “Accurate Modeling of Battery Cathode Materials,” *American Chemical Society National Meeting*, Indianapolis, IN, March 2023.

DEPARTMENT SEMINARS

1. Musgrave, C., "Ab Initio Simulations for Film Growth and Polymer Force Fields," *Department of Chemical Engineering Colloquium*, Stanford, CA, April 1994.
2. Musgrave, C., "Development of Molecular Mechanics Potentials and Simulations of Diamond Chemical Vapor Deposition and Nanotechnology," *Department of Materials Science Colloquium*, North Carolina State University, Raleigh, NC, October 1994.
3. Musgrave, C., "Ab Initio Studies of the Manipulation of Reactivity of Surfaces Using STM for Growing Nanostructures and Diamond Chemical Vapor Deposition," Oak Ridge National Laboratory, Oak Ridge, TN, October 1995.
4. Musgrave, C., "Quantum Chemistry of In Situ Doping of Si CVD," *Department of Materials Science and Engineering Colloquium*, Stanford University, Stanford, CA, November 1996.
5. Musgrave, C., "The Adsorption and Decomposition of Phosphine on Si(100)," NASA Moffett Field, Mountain View, CA, March 1997.
6. Musgrave, C., "Ab Initio Simulations of Semiconductor Processing Chemistry," *Department of Chemical Engineering Colloquium*, Stanford, CA, March 1999.
7. Musgrave, C., "Cluster Simulations of Silicon Surface Chemistry: Is Charge Transfer a Non-local Effect?," Lawrence Livermore National Laboratory, Livermore, CA, May 1999.
8. Musgrave, C., "Prediction of Chemical Mechanisms for Semiconductor Processing," *Department of Chemical Engineering Colloquium*, University of Illinois, Urbana, IL, February 2000.
9. Widjaja, Y., and C. Musgrave, "Silicon Nitride Deposition Using Ammonia," *Department of Chemical Engineering*, Stanford University, Stanford, CA, October 2000.
10. Senosiain, J., C. Musgrave, D. M. Golden, "Reaction of OH and O (3-P_J) with H₂O₂: A Comparative Study," *National Institute of Standards and Technology International Symposium on Kinetics*, Washington, D.C., July 2001.
11. Musgrave, C., "The Chemical Mechanisms of High-K Gate Stack Film Deposition," Lawrence Livermore National Laboratory, Livermore, CA, January 2002.
12. Musgrave, C., "Quantum Chemical Studies of Semiconductor Processing," *Department of Chemical Engineering Colloquium*, University of Florida, March 2002.
13. Musgrave, C., "Quantum Chemical Predictions of the Chemical Mechanisms of High-K Gate Stack Film Deposition," *Department of Materials Science and Engineering Colloquium*, Stanford University, Stanford, CA, April 2002.
14. Musgrave, C., "The Chemical Mechanisms of High-K Gate Stack Film Deposition," *Department of Chemical Engineering Colloquium*, University of California, Santa Barbara, CA, May 2002.
15. Prinz, F., C. Musgrave, "Low Temperature Solid Oxide Fuel Cells," *Department of Mechanical Engineering Colloquium*, New Jersey Institute of Technology, Newark, NJ, September 2002.

16. Musgrave, C., "A Chemically Accurate DFT Method and Quantum Chemical Predictions of the Chemical Mechanisms of High-K Gate Stack Film Deposition," Sandia National Laboratory, Sandia, NM, September 2002.
17. Musgrave, C., "A Chemically Accurate DFT Method and Quantum Chemical Predictions of the Chemical Mechanisms of High-K Gate Stack Film Deposition," *Department of Chemistry Physical Chemistry Seminar*, Colorado State University, Fort Collins, CO, September 2002.
18. Musgrave, C., "A Chemically Accurate DFT Method and Quantum Chemical Predictions of the Chemical Mechanisms of High-K Gate Stack Film Deposition," *Department of Chemical Engineering Colloquium*, Massachusetts Institute of Technology, Cambridge, MA, September 2002.
19. Musgrave, C., "A Chemically Accurate DFT Method and Quantum Chemical Predictions of the Chemical Mechanisms of High-K Gate Stack Film Deposition," *Department of Chemical Engineering Colloquium*, Cornell University, Ithaca, NY, September 2002.
20. Musgrave, C., "A Chemically Accurate DFT Method and Quantum Chemical Predictions of the Chemical Mechanisms of High-K Gate Stack Film Deposition," *Department of Chemical Engineering Colloquium*, Princeton University, Princeton, NJ, September 2002.
21. Musgrave, C., "A Chemically Accurate DFT Method and Quantum Chemical Predictions of the Chemical Mechanisms of High-K Gate Stack Film Deposition," *Surface Science Seminar, Department of Chemistry*, Rutgers University, Piscataway, NJ, September 2002.
22. Musgrave, C., "A Chemically Accurate DFT Method and Quantum Chemical Predictions of the Chemical Mechanisms of High-K Gate Stack Film Deposition," *Department of Chemical Engineering Colloquium and MRSEC Seminar*, University of Wisconsin, Madison, WI, September 2002.
23. Musgrave, C., "Atomistic Simulations of Surface Chemical Reactions for Growing High-K Gate Stacks," *Department of Chemistry Physical Chemistry Seminar*, University of Colorado, Boulder, CO, September 2002.
24. Musgrave, C., "Atomistic Simulations of Surface Chemical Reactions for Growing High-K Gate Stacks," *Department of Chemical Engineering Colloquium*, University of Minnesota, Minneapolis, MN, September 2002.
25. Musgrave, C., "Atomistic Simulations of Surface Chemical Reactions for Growing High-K Gate Stacks," *Special Seminar, Department of Chemistry*, Harvard University, Cambridge, MA, September 2002.
26. Musgrave, C., "Atomistic Simulations of Surface Chemical Reactions for Growing High-K Gate Stacks," *Department of Chemical Engineering Colloquium*, Yale University, New Haven, CT, September 2002.
27. Musgrave, C., "Atomistic Simulations of Surface Chemical Reactions for Growing High-K Gate Stacks," *Department of Chemical Engineering Colloquium*, University of Texas, Austin, TX, September 2002.

28. Musgrave, C., "Atomistic Simulations of Surface Chemical Reactions for Growing High-K Gate Stacks," *Department of Chemical Engineering Colloquium*, California Institute of Technology, Pasadena, CA, October 2002.
29. Musgrave, C., "A Chemically Accurate DFT Method and Quantum Chemical Predictions of the Chemical Mechanisms of High-K Gate Stack Film Deposition," *Department of Chemical Engineering Colloquium*, University of California, San Diego, San Diego, CA, October 2002.
30. Prinz, F., C. Musgrave, "Low Temperature Solid Oxide Fuel Cells," *Department of Mechanical Engineering Colloquium*, Ohio State University, Columbus, OH, October 2002.
31. Musgrave, C., "Quantum Chemical Simulations of Atomic Layer Deposition," *Physical Chemistry Seminar, Stanford University*, Stanford, CA, October 2002.
32. Musgrave, C., "Quantum Simulations of Fabricating Nanostructures," Materials Research Laboratory, California Institute of Technology, Pasadena, CA, November 2002.
33. Musgrave, C., "Atomic Layer Deposition of Advanced Dielectrics," *Department of Chemical Engineering Colloquium*, Stanford, CA, February 2003.
34. Musgrave, C., "Atomic Layer Deposition of Electronic Materials," *Department of Chemical Engineering Colloquium*, University of Illinois, Urbana, IL, September 2003.
35. Musgrave, C., "Chemical Mechanisms for ALD and CVD of Silicon Nitride," *Torrex Corporation*, Livermore, CA, December 2003.
36. Musgrave, C., "Atomic Layer Deposition of Dielectric Materials," *Chemical Division Colloquia*, Naval Research Laboratory, Washington, DC, December 2003.
37. Musgrave, C., "Quantum Simulations of Atomic Layer Deposition for Advanced Microelectronics," *Department of Chemical Engineering Colloquium*, North Carolina State University, Raleigh, NC, January 2004.
38. Musgrave, C., "Atomic Layer Deposition of Novel Materials for Future Nanoelectronics," *Department of Chemical Engineering Colloquium*, University of Florida, March 2004.
39. Musgrave, C., "Quantum Simulations of High-K ALD," Condensed Matter Physics Seminar, Department of Physics, Harvard University, Cambridge, MA, October 2004.
40. Musgrave, C., "The Surface Chemistry of Metal Oxides and Metal Nitrides," Special Seminar, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, December 2004.
41. Musgrave, C., "Chemical Mechanisms of Atomic Layer Deposition of Metal Oxides and Metal Nitrides," *Department of Chemical Engineering Seminar*, University of Rhode Island, Kingston, RI, December 2004.
42. Musgrave, C., "The Chemistry of Atomic Layer Deposition of Metal Oxides and Metal Nitrides," *Department of Chemistry and Chemical Biology Special Seminar*, Harvard University, Cambridge, MA, December 2004.
43. Musgrave, C., "Computational Prototyping of Atomic Layer Deposition for Advanced Materials and Nanotechnology," *Department of Chemical Engineering Colloquium*, University of California, Irvine, CA, March 2005.

44. Musgrave, C., "Quantum Chemical Simulations of Atomic Layer Deposition of Advanced Materials," *Department of Chemical Engineering Colloquium*, University of California, Los Angeles, CA, March 2005.
45. Musgrave, C., "Applications of Atomic Layer Deposition in Nanotechnology," *Stanford-Seoul National University Joint Symposium*, Stanford University, Stanford, CA, June 2005.
46. Musgrave, C., "Quantum Chemical Studies of Atomic Layer Deposition and Molecular Electronics," *Department of Chemistry Seminar*, University of Seville, Seville, Spain, July 2005.
47. Musgrave, C., "Quantum Simulations as an Engineering Tool for Computational Prototyping of Molecular Processes; Atomic Layer Deposition, Fuel Cell Catalysts, Solar Cell Dyes and Molecular Electronics," *Department of Chemistry Chemical Physics Seminar*, University of Delaware, Newark, DE, September 2005.
48. Musgrave, C., "Theoretical Surface Chemistry: Organic Functionalization of Surfaces and Atomic Layer Deposition of Advanced Materials," *Surface Science Seminar*, Departments of Chemistry and Physics, Rutgers University, Piscataway, September 2005.
49. Musgrave, C., "Atomistic Simulations of Atomic Layer Deposition," *Department of Chemistry Seminar*, Centre National De La Recherche Scientifique, Toulouse, France, January 2006.
50. Musgrave, C., "Quantum Chemical Simulations as a Tool for Computational Prototyping of Molecular Processes," *Department of Chemical Engineering Seminar*, Brigham Young University, Provo UT, January 2006.
51. Musgrave, C., "Quantum Simulations of High-K Deposition and Interfaces," *Department of Chemical Engineering Seminar*, University of New Mexico, Albuquerque NM, September 2006.
52. Musgrave, C., "Molecular Design of Homogeneous Catalysts for Methane to Methanol Conversion, Enantioselective Epoxide Ring Opening and Other Valuable Transformations," *Department of Chemical Engineering Colloquium*, Stanford University, Stanford, CA, December, 2006.
53. Musgrave, C., "Quantum Simulations for Computational Prototyping of Molecular Processes; Atomic Layer Deposition and Methane to Methanol Catalysis," *Department of Chemical Engineering Colloquium*, University of Colorado, Boulder, CO, February, 2007.
54. Musgrave, C., "Molecular Design of Homogeneous Catalysts," *Department of Chemical Engineering Colloquium*, Colorado School of Mines, Golden, CO, January 2008.
55. Musgrave, C., "Computational Prototyping of Chemically Reacting Systems Using Quantum Chemical Simulations: Atomic Layer Deposition and Homogeneous Catalysis," *Department of Chemical Engineering Colloquium*, University of Colorado, Boulder, CO, January 2009.
56. Paul, A., P. Zimmerman, and C. Musgrave, "Quantum Chemical Study of Pathways for Ammonia-Borane Dehydrogenation by Homogeneous Catalysts," Peking University, Beijing, China, March, 2009.

57. Paul, A., P. Zimmerman, and C. Musgrave, "Concerted Pathways of Ammonia-Borane Dehydrogenation: A Rare Case of Tandem Catalysis?," Institute of Theoretical and Computational Chemistry, Nanjing University, Nanjing, China, March 2009.
58. Paul, A., P. Zimmerman, C. Musgrave, "A Computational Perspective of Chemical Hydrogen Storage," Fudan University, Shanghai, China, March 2009.
59. Zimmerman, P., Paul, A. and Musgrave, C., "Quantum Simulations of Ammonia Borane Dehydrogenation Catalysts for Hydrogen Storage," *Chemical Physics Seminar*, Department of Chemistry, University of Colorado, Boulder, CO, April 2009.
60. Musgrave, C., P. Zimmerman and Z. Zhang, "Singlet Fission in Conjugated Molecular Organic Materials: Polyacenes, Graphene and Carbon Nanotubes," Department Seminar, Korean Advanced Institute of Science and Technology, Daejeon, South Korea, June 2010.
61. Musgrave, C., A. Holder, P. Zimmerman and Z. Zhang, "Singlet Fission in Conjugated Molecular Organic Materials," Physical Chemistry Seminar, Department of Chemistry, Colorado State University, April 2011.
62. Musgrave, C., A. Holder, P. Zimmerman and Z. Zhang, "Singlet Fission in Organic Photovoltaic Materials Mediated by Dark Multiexcitonic States," National Renewable Energy Laboratory, Golden, CO, May 2011.
63. Musgrave, C., "Quantum Simulations for Energy Applications: Carrier Multiplication in Organic Photovoltaics and Catalytic Reduction of CO₂," Department Seminar, Department of Chemical Engineering, Brigham Young University, September 2011.
64. Musgrave, C., "Quantum Simulations of Catalytic, Photochemical and Photovoltaic Processes," Department Seminar, Department of Chemical Engineering, University of Pittsburg, February 2014.
65. Musgrave, C., "The Catalytic Reduction of CO₂ to Methanol," Department Seminar, Department of Chemistry, Tulane University, March 2014.
66. Musgrave, C., "Materials for Energy Conversion," Seminar, Department of Chemical and Biological Engineering, University of Colorado Boulder, March 2014.
67. Holder, A., K. Osborn, C. Lobb, and C. Musgrave, "Role of Defects in Metal Oxides for Applications in Quantum Computing and Charge Storage", *National Renewable Energy Laboratory*, Golden, CO, October, 2014.
68. Musgrave, C., "Organic Catalysts and Photocatalysts," Department Seminar, Department of Chemistry, Brigham Young University, November 2015.
69. Lim C.H., A.M. Holder, J.T. Hynes, and C.B. Musgrave, "Renewable Organo Hydrides for Catalytic Reduction of CO₂ to Fuels," *National Renewable Energy Laboratory*, Golden, CO, February, 2016.
70. Musgrave, C., "Organic Photocatalysts for Photopolymerizations – Powerful Photoredox Reducing Agents Driven by Visible Light," *Department of Chemistry and Center for Photochemical Sciences, Bowling Green State University*, Bowling Green, OH, September 2016.

71. Musgrave, C., "Organic Photocatalysts - Powerful Photoredox Reducing Agents Driven by Visible Light," *Department of Chemical Engineering, University of California, Riverside*, October 2016.
72. Musgrave, C., "Organic Catalysts and Photocatalysts - Powerful and Renewable Reducing Agents," *Department of Chemical Engineering, Yale University, New Haven, CT*, November 2016.
73. Musgrave, C., "Ab Initio Design of Organic Photoredox Catalysts for Atom Transfer Radical Polymerization," *Department of Chemical Engineering, University of Wisconsin, Madison, WI*, March 2017.
74. Musgrave, C., "Ab Initio and Machine Learned Design of Molecular and Solid Catalysts," *Department of Chemical Engineering, University of New Mexico, Albuquerque, NM*, April 2018.
75. Musgrave, C., "Marrying Machine Learning and Ab Initio Methods to Design Molecular and Solid Catalysts," *Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA*, April 2018.
76. Musgrave, C., "Computational Design of Organic Catalysts and Photocatalysis," *Department of Chemical Engineering, University of Oklahoma, OK*, September 2018.
77. Musgrave, C., "Machine Learning and Ab Initio Methods to Discover and Design Novel Materials and Catalysts," *Department of Chemical Engineering, Georgia Institute of Technology, Atlanta, GA*, October 2018.
78. Musgrave, C., "Computational Design of Organic Catalysts and Photocatalysis for ATRP and CO₂ Reduction," *Department of Chemistry, King Abdullah University of Science and Technology, Thuwai, Saudi Arabia*, October 2018.
79. Musgrave, C., "Machine Learning and Ab Initio Methods to Discover and Design Novel Materials and Catalysts," *Department of Chemical Engineering, University of Massachusetts, Amherst, MA*, December 2018.
80. Musgrave, C., "Computational Design of Organic Catalysts and Photocatalysis," *The Ohio State University, Columbus, OH*, January 2019.
81. Musgrave, C., "Ab Initio and Machine Learned Modeling for the Design and Discovery of New Materials for Energy Applications," *Air Force Research Laboratories, Dayton, OH*, January 2019.
82. Musgrave, C., "Accelerating the Discovery of New Materials for Energy Applications Using Ab Initio and Machine Learned Modeling," *Department of Chemical and Biomolecular Engineering, New York University, New York, NY*, November 2019.
83. Musgrave, C., "Ab Initio and Machine Learned Modeling for Accelerated Discovery of Catalysts and Materials," *Department of Chemical Engineering, University of South Florida, Tampa, FL*, December 2019.
84. Musgrave, C., "Accelerated Discovery of New Materials for Energy Applications using Quantum Simulations in Partnership with Machine Learning," *Materials Science and Engineering, University of Wyoming, Laramie, WY*, April 2020.

85. Musgrave, C., “Accelerated Discovery of Materials using Quantum Simulations and Machine Learning,” *Materials Science and Engineering, University of Colorado*, Boulder, CO, August 2022.
86. Musgrave, C., “More Accurate Modeling of Electrochemistry Using Grand Canonical Quantum Chemistry,” *Department of Chemistry, Rutgers University*, New Brunswick, New Jersey, October 2022.
87. Musgrave, C., “Accurate Modeling of Electrocatalysis Using Grand Canonical Quantum Chemistry,” *Department of Chemical Engineering, Pennsylvania State University*, State College, PA, January 2023.

INVITED INDUSTRY SEMINARS

1. Musgrave, C., “Ab Initio Simulations of Phosphine Adsorption on Silicon (100) 2x1,” Xerox Palo Alto Research Center, Palo Alto, CA, May 1997.
2. Musgrave, C., “Cluster Simulations of Surface Reactions for Semiconductor Processing,” LSI Logic, Santa Clara, CA, September 1999.
3. Musgrave, C., “The Atomic Layer Deposition of ZrO₂ and HfO₂ High-K Dielectrics,” Novellus, Santa Clara, CA, June 2002.
4. Musgrave, C., “Quantum Chemical Simulations of Nitridization and Oxidation of Silicon,” Intel Corp., Santa Clara, CA, September 2002.
5. Musgrave, C., “Atomic Layer Deposition of ZrO₂ and HfO₂ High-K Dielectrics,” Motorola, Inc. Austin, TX, September 2002.
6. Musgrave, C., “Density Functional Theory Study of Atomic Layer Deposition of High-K Dielectrics for Future MOSFETs,” Intel Corp., Santa Clara, CA, December 2002.
7. Musgrave, C., “Simulation of ALD of High-K Thin Films Using Metal Chlorides and Metal Alkylamides,” Applied Materials Corporation, Santa Clara, CA, May 2003.
8. Musgrave, C., “Computational Prototyping of High-K Dielectric Deposition by ALD Using Density Functional Theory Simulations,” Novellus Corporation, Santa Clara, CA, July 2003.
9. Musgrave, C., “ALD for Deposition of Nanostructured Electronic Materials,” Nanosys Corporation, Menlo Park, CA, December 2003.
10. Musgrave, C., “Chemical Mechanisms for ALD and CVD of Silicon Nitride,” Torrex Corporation, Livermore, CA, December 2003.
11. Musgrave, C., “Surface Functionalization for Atomic Layer Deposition,” Cabot Corporation, Billerica, MA, May 2004.
12. Musgrave, C., “New Materials for Integrated Circuits,” KLA-Tencor Corporation, Milpitas, CA, September 2004.
13. Musgrave, C., “Chemical Mechanisms of Atomic Layer Deposition,” Aixtron-Genus, Sunnyvale, CA, September 2005.
14. Musgrave, C., “Quantum Molecular Dynamics Simulations of HfO₂ Atomic Layer Deposition for High-K Gate Applications,” Intel, Santa Clara, CA, March 2007.

15. Musgrave, C., "Quantum Simulations of Electronic Materials Processing for Microelectronics Fabrication," Applied Materials Corporation, Santa Clara, CA, October 2011.
16. Musgrave, C., "Guidelines for Computationally Accelerated Discovery of Materials," Applied Materials Corporation, Santa Clara, CA, November 2016.

CONFERENCE PRESENTATIONS

1. Musgrave, C., "Development of Molecular Mechanics Potentials from First Principles: The Si(111)-7x7 Reconstruction," *West Coast Theoretical Chemistry Conference*, Salt Lake City, UT, May 1990.
2. Musgrave, C., "Molecular Mechanics Simulations of the Dimer Adatom Stacking Fault (2n+1) x (2n+1) Reconstructions of (111) Silicon," *American Conference of Theoretical Chemistry*, San Diego, CA, June 1990.
3. Musgrave, C., "A Hydrogen Abstraction Tool for Nanotechnology," *Foresight Conference on Nanotechnology*, Palo Alto, CA, November 1991.
4. Musgrave, C., "Ab Initio Simulations of the Chemical Vapor Deposition of Diamond," *West Coast Theoretical Chemistry Conference*, Mountain View, CA, May 1992.
5. Musgrave, C., and M. Mysinger, "First Principles Study of Phosphine Adsorption and Decomposition on Si(100)-2x1," *American Institute of Chemical Engineers Annual Meeting*, Miami, FL, November 1998.
6. Musgrave, C., "Adhesion, Dynamics and Degradation of PFPE Hard Disk Lubricants," Center on Polymer Interfaces and Macromolecular Assemblies (CPIMA) Forum, Department of Chemical Engineering, Stanford University, Stanford, CA, August 1999.
7. Ricca, A., and C. Musgrave, "Modeling Silicon Surface Chemistry with Clusters: Chlorine on the Si(100)-2x1 and (111) Surfaces," *American Institute of Chemical Engineers Annual Meeting*, Miami, FL, November 1998.
8. Mysinger, M., A. Ricca, and C. Musgrave, "A Quantum Chemical Study of the Chemistry of Silicon Surfaces: Cl, Phosphine and Ammonia on Silicon," *American Institute of Chemical Engineers Annual Meeting*, Miami, FL, November 1998.
9. Senosiain, J., D. Golden, and C. Musgrave, "Use of Ab Initio Quantum Mechanics To Estimate Rate Constants," US-German Environmental Chamber Workshop, University of California, Riverside, CA, October 1999.
10. Mui, C., S. Bent, and C. Musgrave, "Theoretical Approach for Predicting Si_{x-1}Ge_x Surface Chemistry," *American Institute of Chemical Engineers Annual Meeting*, Dallas, TX, November 1999.
11. Kang, J., and C. Musgrave, "The KMLYP Density Functional Approximation: A New Method for Accurate Prediction of Activation Barriers and Enthalpies of Reaction," *AVS 48th International Symposium*, Boston, MA, October 2000.

12. J. Kang, and C. Musgrave, "A New Method for the Accurate Prediction of Activation Barriers and Enthalpies of Reaction, American Institute of Chemical Engineering," Los Angeles, CA, November 2000.
13. Senosiain, J., D. Golden, J. Kang, and C. Musgrave, "Use of Ab Initio Quantum Methods and Transition State Theory to Estimate Rate Constants for Computational Prototyping," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.
14. Kang, J. and C. Musgrave, "A Theoretical Study of the Chemical Vapor Deposition of (100) Diamond: An Explanation for the Slow Growth of the (100) Surface," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.
15. Mui, C., S. Bent, and C. Musgrave, "Theoretical Predictions for SiGe Heteroepitaxy," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.
16. Widjaja, Y. and C. Musgrave, "Quantum Chemical Study of Silicon Nitride Deposition Using Ammonia," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.
17. Kang, J. and C. Musgrave, "The KMLYP Hybrid DFT Method: A Chemically Accurate Method for Understanding Reactivity," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.
18. Widjaja, Y. and C. Musgrave, "An Ab Initio Study of the Initial Oxidation of the Silicon (100)-2x1 Surface," *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.
19. Widjaja, Y. and C. Musgrave, "An Ab Initio Study of the Initial Oxidation of Si(100)-(2x1)," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.
20. Musgrave, C. and J. Kang, "A Theoretical Study Of The Chemical Vapor Deposition Of (100) Silicon From Silane," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.
21. Musgrave, C. and Y. Widjaja, "Quantum Chemical Study of Zirconium Oxide Atomic Layer Deposition: Gas Phase and Surface Reactions," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.
22. Musgrave, C. and J. Kang, "Nanometer Scale Manipulation of Surface Reaction Kinetics by STM Electric Fields: A Density Functional Theory Study," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.
23. C. Musgrave, "Teaching Quantum Chemical Simulations in Chemical Engineering," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.
24. Kang, J. and C. Musgrave, "Prediction of Accurate Reaction Barriers and Enthalpies of Reaction by a New Hybrid DFT Method," Poster Presentation, *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.
25. Senosiain, J., D. Golden, and C. Musgrave, "Tunneling Effects in Bimolecular Chemical Reactions," Poster Presentation, *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

26. Prinz, P. and C. Musgrave, "Low Temperature Solid Oxide Fuel Cells," *2002 Office of Naval Research: Materials Review*, Woods Hole, MA, May 2002.
27. Widjaja, Y. and C. Musgrave, "Quantum Simulations of Growth of High-K Gate Stacks," *American Institute of Chemical Engineers Annual Meeting*, Indianapolis, IN, November 2002.
28. Mui, C., C. Musgrave, and S. Bent, "Hydrogen Desorption from (100) 2x1 Silicon, Germanium and SiGe Alloy Surfaces," *American Institute of Chemical Engineers Annual Meeting*, Indianapolis, IN, November 2002.
29. Mui, C. and C. Musgrave, and S. Bent, "Organic Functionalization of Silicon and Germanium Surfaces," *American Institute of Chemical Engineers Annual Meeting*, Indianapolis, IN, November 2002.
30. Senosiain, J., J. Kang, D. Golden, and C. Musgrave, "A Critical Analysis of Quantum Chemical Methods for the Prediction of Kinetics and Thermochemical Properties," *American Institute of Chemical Engineers Annual Meeting*, Indianapolis, IN, November 2002.
31. Musgrave, C. and J. Han, "ALD of High-K Gate Materials on Si, Ge and SiGe Alloy Materials for 3-D Microelectronics," MARCO Materials, Structures and Devices Center Teleconference, Massachusetts Institute of Technology, Cambridge, MA, April 2003.
32. Musgrave, C., Y. Widjaja, and J. Han, "Atomistic Simulations of Surface Chemical Reactions for Growing High-K Gate Stacks," Materials Research Society Spring Meeting, San Francisco, CA, April 2003.
33. Musgrave, C., "Quantum Chemical Simulations for Nanoelectronics: Materials by Design," *NSF Nanoscience Young Scientist Exchange Program*, Tokyo University, Tokyo, Japan, November 2003.
34. Xu, Y., and C. Musgrave, "Quantum Simulation of Thin Film Growth for 3D Microelectronic Devices," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.
35. Musgrave, C., "ALD of High-K Dielectrics with Alkylamide Precursors," *MARCO Materials Structures and Devices Center Review*, Massachusetts Institute of Technology, Cambridge, MA, April 2004.
36. Han, J., M. Kelly, C. Musgrave and G. Parsons, "DFT Study of the Initial ALD Reactions of $\text{Hf}(\text{N}(\text{CH}_3)_2)_4$ on the Si-H Surface: Chemical Mechanism and Vibrational Spectra," *The Fourth American Vacuum Society Topical Conference on Atomic Layer Deposition*, Helsinki, Finland, August 2004.
37. Han, J. and C. Musgrave, "Quantum Chemical Simulations of ALD of HfO_2 Using Hafnium Alkylamide Precursors," *The Fourth American Vacuum Society Topical Conference on Atomic Layer Deposition*, Helsinki, Finland, August 2004.
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39. Mui, C. and C. Musgrave, "A Comparison of the Surface chemistry of Si and Ge: H Desorption, Oxidation, Nitridation and Organic Functionalization," *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.
40. Han, J., M. Kelly, G. Parsons and C. Musgrave, "DFT Study of the Initial ALD Reactions of $\text{Hf}(\text{N}(\text{CH}_3)_2)_4$ on the SiO_2 and Si-H Surfaces: Mechanism, Kinetics, Vibrational Spectra and Interface Structure," *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.
41. Xu, Y. and C. Musgrave, "ALD of High-K Dielectrics on Nitrided Si and Ge Surfaces," *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.
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46. Dupont, G. and C. Musgrave, "Electronic Coupling of Organics to Semiconductors Through Quantum Resonance," *American Physical Society March Meeting*, Los Angeles, CA, March 2005.
47. Han, J. and C. Musgrave, "Density Functional Theory Simulations of Atomic Layer Deposition of HfO_2 ," *American Physical Society March Meeting*, Los Angeles, CA, March 2005.
48. Dupont, G. and C. Musgrave, "DFT Study of Amino Acids on Si Surface for Hybrid Organic-Semiconductor and Protein-Semiconductor Structures," *American Physical Society March Meeting*, Los Angeles, CA, March 2005.
49. Mui, C. Y. Xu, and C. Musgrave, "DFT Simulations of the Growth of Thin Films on Si and Ge," *American Physical Society March Meeting*, Los Angeles, CA, March 2005.
50. Dupont, G. and C. Musgrave, "Organic Functionalization of Semiconductors Using Amino Acids: Quantum Resonance Coupling and Electron Transport Effects," *American Vacuum Society Annual Meeting*, Boston, MA, November 2005.
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55. Dupont, G., P. Ardalán, and C. Musgrave, "Reactions of Amino Acids on Si and Ge Surfaces", *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
56. Mukhopadhyay, A., J. Sanz and C. Musgrave, "The Electronic Structure of Metals on High-K Dielectrics; Metal Induced Gap States for the Ru and RuO_2 on HfO_2 Interfaces," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
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58. Xu, Y., A. Mukhopadhyay and C. Musgrave, "Prediction of Reaction Kinetics in ALD of Metal Oxides and Nitrides," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
59. Paul, A. and C. Musgrave, "A Detailed Theoretical Study of the Mechanism and Energetics of Methane to Methanol Conversion by Cis-Platin and Catalytica," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
60. Han, J., K. Huang, R. Waymouth, A. Paul and C. Musgrave, "Ab Initio Molecular Design of Catalysts for Ethylene and Styrene Polymerization and Methane to Methanol Conversion," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
61. Widjaja, Y., C. Mui, A. Mukhopadhyay and C. Musgrave, "The Role of Dative Bonding in the Reactivity of Semiconductor and Metal Oxide Surfaces," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
62. C. Musgrave, "Ab Initio Simulations of Surface Chemistry for Thin Film Growth of Electronic Materials," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
63. Zhang, G. and C. Musgrave, "Accurate Prediction of Electron Transport across Organic-Semiconductor Junctions," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
64. Zimmerman, P., A. Paul, Z. Zhang and C. Musgrave, "First Principles Description of Dark Multi-Exciton States Involved in MEG of Carbon Nanotubes," *American Chemical Society Spring National Meeting*, San Francisco, CA, March 2010.
65. Musgrave, C., A. Holder, P. Zimmerman and Z. Zhang, "Singlet Fission in Conjugated Molecular Organic Materials for High Efficiency Organic Photovoltaics," *Center for Revolutionary Solar Photoconversion Annual Meeting*, Colorado State University, Fort Collins, CO, September 2010.

66. Holder, A., and C. Musgrave, "Quantum Chemical Simulations of Two-Level Systems in Atomic Layer Deposited Al₂O₃ Coherent Superconducting Phase Qubit Dielectrics," *Coherent Superconducting Qubit Meeting*, San Diego, CA, January, 2011.
67. Musgrave, C., C. Lim and A. Holder, "Aromatic Stabilization as a Design Principle for Electro- and Photo-electrochemical 1 e⁻ Reduction Catalysts," American Chemical Society Spring National Meeting, New Orleans, LA, April, 2013.
68. Lim, C., C. Musgrave and A. Holder, "Mechanistic Studies of the Catalytic Reduction of CO₂ to Methanol," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November, 2013.
69. Musgrave, C., A. Holder, and P. Zimmerman "The Mechanism of Singlet Fission in Pentacene Organic Photovoltaics," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November, 2013.
70. Musgrave, C., C. Lim, T. Gong, A. Holder, and C. Bowman "The Ab Initio Design of Efficient Photoinitiators," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November, 2013.
71. Muhich, Christopher L., Jinjing Qiu, Aaron Holder, Yung-Chien Wu, Alan W. Weimer, Wei Wei, Lisa McElwee-White and Charles B. Musgrave "Solvent Control of Surface Plasmon Mediated Chemical Deposition of Au Nanoparticles from Alkylgold Phosphine Complexes," *American Institute of Chemical Engineers Annual Meeting*, Salt Lake City, UT, November, 2015.
72. Musgrave, C., C. Lim, A. Holder, J. Hynes, "Dihydropteridine/Pteridine As a 2H⁺/2e⁻ Redox Mediator for the Catalytic Reduction of CO₂ to Methanol Via Hydride-Proton Transfer," *American Institute of Chemical Engineers Annual Meeting*, Salt Lake City, UT, November, 2015.
73. Musgrave, C., C. Lim, A. Holder, J. Hynes, "Reduction of CO₂ to Methanol Catalyzed By a Biomimetic Organo-Hydride Produced from Pyridine," *American Institute of Chemical Engineers Annual Meeting*, Salt Lake City, UT, November, 2015.
74. Lim, C., J. Theriot, G. Miyake and C. Musgrave, "Organic Photocatalysts For Atom Transfer Radical Polymerization Driven By Visible Light," *American Chemical Society Spring Meeting*, San Diego, CA, March, 2016.
75. Musgrave, C., C. Lim, J. Theriot, G. Miyake, H. Yang and M. Ryan, "Organocatalyzed Atom Transfer Radical Polymerization Driven By Visible Light," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November, 2016.
76. Musgrave, C., C. Lim, J. Theriot, and G. Miyake, H. Yang and M. Ryan, "Organic Photocatalysts for Atom Transfer Radical Polymerization Driven By Visible Light," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November, 2016.
77. Musgrave, C., C. Lim, G. Miyake, and J. Theriot, "Ab Initio Design of Organic Catalysts and Photocatalysts," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November, 2016.

78. Musgrave, C., C. Lim, J. Theriot, and G. Miyake, H. Yang and M. Ryan, "Design of photoredox catalysts for efficient organocatalyzed atom transfer radical polymerization," *American Chemical Society Spring Meeting*, San Francisco, CA, April, 2017.

STUDENT AND POSTDOC PRESENTATIONS

1. Mysinger, M. and C. Musgrave, "Modeling Silicon Surface Chemistry from First Principles: The Effect of Cluster Size and Constraints, Plus a Comparison to Periodic DFT," *American Institute of Chemical Engineers Annual Meeting*, Miami, FL, November 1998.
2. Mui, C., S. Bent and C. Musgrave, "Theoretical Studies of Cycloaddition Reactions on Semiconductor Alloy Surfaces," *Chemical Reactions at Surfaces, Gordon Research Conference*, March 1999.
3. Wang, G., C. Mui, C. Musgrave and S. Bent, "Cycloaddition of Cyclopentadiene and Dicyclopentadiene on Si(100)-2x1: Comparison of Monomer and Dimer Adsorption," *Physical Electronics Conference*, June 1999.
4. Widjaja, Y., and C. Musgrave, "Ab Initio Study of Adsorption and Decomposition of NH₃ on Si(100)-(2x1)," *AVS 46th International Symposium*, Seattle, WA, October 1999.
5. Kang, J., and C. Musgrave, "The Effect of STM Electric Fields on H Desorption and Chemical Vapor Deposition of (100) Diamond," *AVS 46th International Symposium*, Seattle, WA, October 1999.
6. Mysinger, M. and C. Musgrave, "The Potential Energy Surfaces and Vibrational Spectra of Phosphine Adsorption and Decomposition on Si(100)-2x1," *American Institute of Chemical Engineers Annual Meeting*, Dallas, TX, November 1999.
7. Mui, C., G. Wang, S. Bent, and C. Musgrave, "Cycloaddition of Cyclopentadiene and Dicyclopentadiene on Si(100)-2x1: Comparison of Monomer and Dimer Adsorption," *American Institute of Chemical Engineers Annual Meeting*, Dallas, TX, November 1999.
8. Widjaja, Y., M. Mysinger, and C. Musgrave, "The Adsorption and Decomposition of NH₃ on Si(100)-(2x1) for Silicon Nitride Growth," *1st International AVS Conference on Microelectronics and Interfaces*, February 2000.
9. Mui, C., S. Bent and C. Musgrave; "Organic Nanostructures on SiGe Surfaces," *1st International AVS Conference on Microelectronics and Interfaces*, Santa Clara CA, February 2000.
10. Mysinger, M. and C. Musgrave, "Potential Energy Surfaces And Vibrational Spectra of Phosphine Adsorption and Decomposition on Si(100)-2x1," *American Chemical Society*, San Francisco, CA, March 2000.
11. Senosiain, J., C. Musgrave and D. Golden, "Theoretical Study of Hydrogen Abstraction from Ethane by Small Radicals," *American Chemical Society*, San Francisco, CA, March 2000.
12. Widjaja, Y., M. Mysinger and C. Musgrave, "Ab Initio Study of Adsorption and Decomposition of NH₃ on Si(100)-(2x1)," *American Chemical Society*, San Francisco, CA, March 2000.

13. Centoni, S., T. Lenosky, B. Sadigh, T. Diaz de la Rubia, C. Musgrave, "First-Principles Calculations of Arsenic Diffusion Mechanisms in Silicon", Cosires 2000 5th International Conference on Computer Simulation of Radiation Effects in Solids, University Park, PA, July 2000.
14. Centoni, S., T. Lenosky, B. Sadigh, T. Diaz de la Rubia, C. Musgrave, "First-Principles Calculation of Arsenic Diffusion Mechanisms in Silicon", *Materials Research Society*, San Francisco, CA, 24 April 2000.
15. Wang, G., C. Mui, C. Musgrave and S. Bent, "Reaction of Pyrrole and Pyrrole Derivatives on Si(100) 2x1," *AVS 48th International Symposium*, Boston, MA, October 2000.
16. Widjaja, Y. and C. Musgrave, "Quantum Chemical Study of Silicon Nitride Deposition Using Ammonia," *AVS 48th International Symposium*, Boston, MA, October 2000.
17. Mui, C., S. Bent and C. Musgrave, "Theoretical Predictions for SiGe Heteroepitaxy," *AVS 48th International Symposium*, Boston, MA, October 2000.
18. Wang, G., C. Mui, C. Musgrave and S. Bent, "Reaction of Pyrrole and Pyrrole Derivatives on Si(100)-2x1," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.
19. Mui, C., G. Wang, S. Bent and C. Musgrave, "Si(100) Surface Modification for Environmentally-Benign Selective Atomic Layer Deposition (ALD)," *Annual Retreat NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing*, Stanford CA, August 2001.
20. Kang, J. and C. Musgrave, "First Principles Calculations of SiO₂ Atomic Layer Deposition and Molecular Nanowires on (100) Silicon," Lawrence Livermore National Laboratory October 2001.
21. Senosiain, J. and C. Musgrave, "Thermal Decomposition Mechanisms of (Ba,Sr)TiO₃ Film precursors," *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.
22. Widjaja, Y. and C. Musgrave, "Quantum Chemical Study of Zirconium Oxide Atomic Layer Deposition," *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.
23. Wang, G., C. Mui, C. Musgrave and S. Bent, "Probing the Selectivity of Multifunctional Compounds on Semiconductor Surfaces: Pyrrole and its Derivatives on Si and Ge (100)-2x1," *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.
24. Mui, C., G. Wang, C. Musgrave and S. Bent, "Are Silicon and Germanium Surfaces Chemically Similar? Reactions of Amines," *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.
25. Kang, J. and C. Musgrave, "A Theoretical Study of The Chemical Vapor Deposition of (100) Silicon From Silane," *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.
26. Wang, G., C. Mui, C. Musgrave and S. Bent, "Competition and Selectivity of Organic Reactions on Semiconductor Surfaces," *16th Annual William S. Johnson Symposium in Organic Chemistry*, Stanford University, CA, October 2001.

27. Wang, G., C. Mui, C. Musgrave and S. Bent, "Probing the Reactivity of Amines on Si(100)-2x1 and Ge(100)-2x1 Surfaces," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.
28. Musgrave, C. and Y. Widjaja, "A DFT Study of the Initial Growth Mechanism of Silicon Nitride on Si(100)-(2x1) Using Ammonia and Atomic Nitrogen," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.
29. Widjaja, Y. and C. Musgrave, Quantum Chemical Study of Zirconium Oxide Atomic Layer Deposition on the Si(100)-(2x1) Surface," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.
30. Wang, G., C. Mui, C. Musgrave and S. Bent, "Competition and Selectivity of Organic Reactions on Semiconductor Surfaces," *5th Annual Flory Conference in Macromolecular and Physical Chemistry*, Stanford, CA, February 2002.
31. Senosiain, J. and C. Musgrave, "Atomic Layer Deposition of High-K Gate Dielectrics on Germanium," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS*, Stanford University, June 2002.
32. Chen, R., Y. Widjaja, G. Gao and C. Musgrave, "Atomic Layer Deposition of High-K Gate Dielectrics," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS*, Stanford University, June 2002.
33. Filler, M., C. Mui, G. Wang, C. Musgrave and S. Bent, "Gaining Molecular and Atomic Level Control of Semiconductor Interfaces through Organic Functionalization," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS*, Stanford University, June 2002.
34. Mui, C., S. Bent and C. Musgrave, "Organic Chemistry at Semiconductor Surfaces Studied by FTIR and DFT," IBM Storage Division, San Jose, CA July 2002.
35. Mui, C., S. Bent and C. Musgrave, "Organic Chemistry at Semiconductor Surfaces Studied by FTIR and DFT," SRI International, Menlo Park CA, December 2002.
36. Senosiain, J., D. Golden and C. Musgrave, "Modeling the kinetics of OH+CO: A Stochastic Approach," Sandia National Laboratory, Livermore, CA, August 2002.
37. Chen, R., C. Mui, S. Bent and C. Musgrave, "Area Selective Atomic Layer Deposition (ALD) of High-K Dielectrics," *Annual Retreat NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing*, Stanford CA, August 2002.
38. Kawakami, B., C. Musgrave, M. Reinhard, and P. Roberts, "Enzyme Reaction Modeling of Hazardous Pollutant Transformation: Structural Basis of Biodegradability," *Biomedical Computation at Stanford Conference*, Stanford University, Stanford, CA, October 2002.
39. Filler, M., C. Mui, C. Musgrave and S. Bent, "Modifying the Semiconductor Interface with Organonitriles," *49th Annual Meeting of the American Vacuum Society*, Denver, CO, November 2002.
40. Chen, R., J. Han, C. Mui, S. Bent and C. Musgrave, "Area Selective ALD of High-K Dielectrics," *Annual Retreat NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing*, Tucson AZ, February 2003.

41. Bent, S., Chen, R., C. Mui and C. Musgrave, "A Theoretical Investigation of Area Selective Atomic Layer Deposition of High-K Dielectrics," *Annual Retreat NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing*, Tucson AZ, February 2003.
42. Chen, R., J. Han, C. Mui, S. Bent, and C. Musgrave, "An Experimental and Theoretical Investigation of Selective Area ALD of High-K Dielectrics," Flory Conference, Stanford, CA, February 2003.
43. Han, J., Y. Widjaja, R. Chen, S. Bent, R. Gordon, G. Gao and C. Musgrave, "A DFT Study of Atomic-Layer Deposition for ZrO_2 and HfO_2 ," Flory Conference, Stanford, CA, February 2003.
44. Huang, K., J. Han, Y. Widjaja, C. Musgrave, and R. Waymouth, "The Role of the Oxidation State of Titanium and Solvent Effects in Ethylene/Styrene Copolymerization: A DFT Theoretical Study," Flory Conference on Novel Electronic Materials, Stanford, CA, February 2003.
45. R. Pornprasertsuk, C. Musgrave and F. Prinz, "DFT Simulations of Oxygen Transport Through ZrO_2 for Low-T Solid Oxide Fuel Cells," Flory Conference, Stanford, CA, February 2003.
46. Xu, Y. and C. Musgrave, "Quantum Simulation of Thin Film Growth for 3-D Microelectronics," Flory Conference on Novel Electronic Materials, Stanford, CA, February 2003.
47. Mui, C., S. Bent and C. Musgrave, "A Theoretical Study on Hydrogen Desorption from SiGe Alloy Surfaces," Flory Conference, Stanford, CA, February 2003.
48. Mui, C., S. Bent and C. Musgrave. "Organic Chemistry at Semiconductor Surfaces Studied by FTIR and DFT," Lam Research Corporation, Fremont CA, May 2003.
49. Han, J., S. Wang, R. Gordon and C. Musgrave, "Kinetics and Thermodynamics of Atomic Layer Deposition of High- κ Dielectrics using Alternative Metallorganic Precursors," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS*, Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.
50. Xu, Y. and C. Musgrave, "Quantum simulation of Thin Film Growth for 3-D Microelectronic Device," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS*, Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.
51. Heyman, A. and C. Musgrave, "Density Functional Theory Calculations of Atomic Layer Deposition of Al_2O_3 from AlCl_3 and H_2O Precursors," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS*, Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.
52. Mui, C., J. Han and C. Musgrave, "Quantum Chemical Studies of Atomic Layer Deposition of Hafnium Oxide," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS*, Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.
53. Chen, R., H. Kim, C. Musgrave, P. McIntyre and S. Bent, "Surface Modification for Area-Selective Atomic Layer Deposition," *Nano and Bio-Nanoscience Research Meeting*,

Northern California Chapter of the AVS, Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.

54. Mui, C., S. Bent and C. Musgrave, "Organic Chemistry at Semiconductor Surfaces Studied by FTIR and DFT," Hitachi Global Storage Technologies, San Jose CA, June 2003.
55. Mui, C. and C. Musgrave, "Quantum Chemical Studies of Atomic Layer Deposition of Hafnium Oxide," Novellus Systems Incorporated, San Jose CA, June 2003.
56. Mui, C. and C. Musgrave, "Quantum Chemical Studies of ALD of Hafnium Oxide Using Alkoxide Precursors," Applied Materials Corporation, San Jose CA, July 2003.
57. Mui, C. and C. Musgrave, "Atomic Layer Deposition of Hafnium Oxide Using Alkoxide Precursors," Intel Corporation, San Jose CA, July 2003.
58. Han, J., S. Wang, R. Gordon, and C. Musgrave, "Atomic Layer Deposition of High-k Dielectrics using Alternative Metallorganic Precursors," *Initiative for Nanoscale Materials Processing Metal Gate-Metal Workfunction Meeting*, Stanford University, Stanford, CA, August 2003.
59. Xu, Y. and C. Musgrave, "ALD of Metals and Metal Oxides on Organics for Organic and Molecular 3D Electronics," *Nano and Bio-Nanoscience Research Meeting, Initiative for Nanoscale Materials Processing Metal Gate-Metal Workfunction Meeting*, Stanford University, Stanford, CA, August 2003.
60. Heyman, A. and C. Musgrave, "DFT Study of ALD of Al_2O_3 from AlCl_3 and H_2O Precursors," *Initiative for Nanoscale Materials Processing Metal Gate-Metal Workfunction Meeting*, Stanford University, Stanford, CA, August 2003.
61. Mui, C., J. Han and C. Musgrave, "Atomic Layer Deposition of Hafnium Oxide Using Alkoxides," *Initiative for Nanoscale Materials Processing Metal Gate-Metal Workfunction Meeting*, Stanford University, Stanford, CA, August 2003.
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181. Hoskins, A., S. L. Millican, C. Czernik, M. Wallace, I. Al-Shankiti, J. Netter, C. B. Musgrave and A. W. Weimer, "Near-Isothermal on-Sun Demonstration to Split Water," *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November 2017.
182. Bartel, C. J., R. O'Toole, M. Kodas, S. Ricote, N. P. Sullivan, A. Drake, A. Horrell, R. Hall, C. B. Musgrave and A. W. Weimer, "Atomically Deposited Sintering Aids: Assessing the Effects of Al₂O₃ Particle ALD on the Sintering and Performance of SOFC Electrolytes," *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November 2017.

183. Clary, J. M., S. A. Van Norman, Dong Su, E. A. Stach, J. L. Falconer, C. B. Musgrave and A. W. Weimer, "Influence of Alumina Support Crystallinity on ALD-Synthesized Cobalt Catalysts for Fischer-Tropsch Synthesis," *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November 2017.
184. Millican, S. L., A. Hoskins, C. Czernik, M. Wallace, I. Al-Shankiti, J. Netter, C. B. Musgrave and A. W. Weimer, "On-Sun Demonstration of Hydrogen Production Via Solar Thermochemical Water Splitting," *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November 2017.
185. Bartel, C. J., R. O'Toole, M. Kodas, S. Ricote, N. P. Sullivan, A. Drake, A. Horrell, R. Hall, C. B. Musgrave and A. W. Weimer, "Effects of Alumina Incorporation by Particle Atomic Layer Deposition on Sintering, Microstructure, and Ionic Conductivity of Yttria-Stabilized Zirconia (8YSZ)," *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November 2017.
186. Bartel, C. J., J. R. Rumpitz, A. M. Holder, A. W. Weimer and C. B. Musgrave, "Screening Binary Redox Pairs for Solar Thermochemical Ammonia Synthesis Using Machine Learned Predictions of Gibbs Formation Energies at Finite Temperatures," *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November 2017.
187. Clary, J. M., S. A. Van Norman, D. Su, E. A. Stach, J. L. Falconer, C. B. Musgrave and A. W. Weimer, "Novel ALD-Formed Cobalt/Alumina Nanostructures Active for Fischer-Tropsch Synthesis," *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November 2017.
188. Millican, S. L., K. Sun, I. Androschuk, A. W. Weimer and C. B. Musgrave, "Assessing the Thermodynamic Viability of Mixed Metal Oxides for Solar Thermochemical Water Splitting," *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November 2017.
189. Kim, K.; J. Sinha, C. Musgrave, and J. Stansbury, "Designing free-radical redox photoinitiators for practical dark curing", *ACS Spring National Meeting*, New Orleans, LA, March 2018
190. Singstock, N., C. Musgrave, A. Holder, "Efficient and Accurate Catalyst Predictions via Machine Learning," International Conference on Ternary and Multinary Compounds, Boulder, CO, September 2018.
191. Bartel, C., C. Sutton, B. Goldsmith, R. Ouyang, C. Musgrave, L. Ghiringhelli, M. Scheffler, "New Tolerance Factor to Predict the Stability of Perovskite Oxides and Halides", *American Institute of Chemical Engineers Annual Meeting*, Pittsburgh, PA, October 2018.
192. Millican, S., I. Androschuk, C. Musgrave and A. Weimer, "Computationally Accelerated Discovery and Experimental Demonstration of Materials for Solar Thermochemical Hydrogen Production," *American Institute of Chemical Engineers Annual Meeting*, Pittsburgh, PA, October 2018.
193. Hoskins, T. Gossett, C. Musgrave and A. Weimer, "Nano-Structured Ceramic ALD Coatings to Stabilize SiC Against Oxidation in High-Temperature Steam Solar Thermal Water Splitting Applications," *American Institute of Chemical Engineers Annual Meeting*, Pittsburgh, PA, October 2018.

194. Millican, S., A Deml, A. Weimer, A. Holder, V. Stevanovic, and C. Musgrave, "Predicting Point Defect Concentrations in Complex, Disordered Oxides," *American Institute of Chemical Engineers Annual Meeting*, Pittsburgh, PA, October 2018.
195. Millican, S., K. Talley, A. Weimer, A. Zakutayev, C. Musgrave, G. Brennecka and A. Holder, "Understanding and Improving the (Al,Sc)N Heterostructural Alloy Through DFT Calculations and Combinatorial Synthesis," *American Institute of Chemical Engineers Annual Meeting*, Pittsburgh, PA, October 2018.
196. Kim, K., J. Sinha, K. Childress, C. Musgrave, and J. Stansbury, "A Fresh Look at Redox Initiation: New Possibilities for High Efficiency Photocuring" 2019 CU Dental Research Day, Aurora CO, February 2019.
197. Kim, K., J. Sinha, K. Childress, C. Musgrave, and J. Stansbury, "Chemically Extended Radical Photopolymerization Beyond Temporal Irradiation Limitations: Radical Dark Curing Photoinitiator," *American Chemical Society Spring Meeting*, Orlando, FL, March 2019.
198. Bartel, C., A. Weimer, S. Lany, C. Musgrave, A. Holder, "Decomposition Reactions Dictate the Performance of First-principles Predictions of Solid-stability," *American Chemical Society Spring Meeting*, Orlando, FL, March 2019.
199. Lim, C., J. Hynes, K. Glusac, C. Musgrave, "Benzimidazoles as Recyclable Metal-free Hydrides for CO₂ Reduction to Formate," *American Chemical Society Spring Meeting*, Orlando, FL, March 2019.
200. Bartel, C., C. Sutton, B. Goldsmith, A. Holder, C. Musgrave, "Computational Identification of All-inorganic Cesium Chloride Double Perovskite Solar Absorbers," *American Chemical Society Spring Meeting*, Orlando, FL, March 2019.
201. Kim, K. C. Musgrave, and J. Stansbury, "Rational Design of Base Amplifiers for Athermal Radical Shadow Curing", *Fundamentals and Applications of photopolymerization - Industry-University Cooperative Research Center Fall Meeting*, Exton, PA, May 2019.
202. Kim, K. N. Singstock, K. Childress, J. Sinha, A. Salazar, S. Whitfield, A. Holder, J. Stansbury, and C. Musgrave, "Rational Design of Efficient Amine Reductant Initiators for Amine-Peroxide Redox Polymerization", *Fundamentals and Applications of photopolymerization - Industry-University Cooperative Research Center Fall Meeting*, Exton, PA, May 2019.
203. Bull, S. K., W. McNeary, C. Adkins, T. Champ, C. Hill, R. O'Brien, C. Musgrave, and A. Weimer, "Particle Atomic Layer Deposition of Tungsten Nitride Environmental Barrier Coatings from Bis(t-butyylimido)bis(dimethylamino)tungsten(VI) and Ammonia." *ALD/ALE 2019* Bellevue, Washington, July 2019.
204. Kim, K. J. Sinha, A. Salazar, G. Gao, S. Whitfield, K. Childress, S. Sartor, P. Shah, E. Wendt, C. Musgrave, and J. Stansbury, "Radical photopolymerization with dark curing: Overcoming intrinsic issue of photopolymerization", *International Conference of Photochemistry*, Boulder, CO, July 2019.
205. Alherz, A., S. Illic, C. Lim, K. Glusac, and C. Musgrave, "Organic Hydrides for the Photoelectrochemical Catalytic Reduction of CO₂", *International Conference of Photochemistry*, Boulder, CO, July 2019.

206. Bare, Z., C. Bartel, S. Millican, A. Holder, C. Musgrave, "Ab Initio and Machine Learned Modeling to Screen and Discover Materials for Solar Thermal Water Splitting", *Digital Solar Redox Materials Design Workshop*, Berkeley CA, August 2019.
207. Kim, K. J. Sinha, G. Gao, P. Shah, K. Childress, S. Sartor, A. Salazar, S. Whitfield, E. Wendt, C. Musgrave, and J. Stansbury, "Solvent-Free Radical Photopolymerization with Dark Curing", *Photopolymerization Fundamentals 2019*, Monterey CA, September 2019.
208. Kim, K., N. Singstock, K. Childress, J. Sinha, A. Salazar, S. Whitfield, A. Holder, J. Stansbury, and C. Musgrave, "Rational Design of Efficient Amine Reductant Initiators for Amine-Peroxide Redox Polymerization", *Student Annual Research Symposium*, Boulder CO, September 2019.
209. Kim, K., J. Sinha, A. Salazar, C. Musgrave, and J. Stansbury, "Dark-Curing Photoinitiators that Extend the Cure Depths in Composite Materials", *Academy of Dental Materials Annual Meeting 2019*, Jackson Hole WY, October 2019.
210. Jenkins, A., C. Musgrave, and J. Medlin, "Improving Thermal Stability of Supported Metal Catalysts Via Phosphonic Acid Self-Assembled Monolayers," *American Institute of Chemical Engineers Annual Meeting*, Orlando, Florida, November 2019.
211. Bull, S., T. Champ, R. O'Brien, C. Musgrave, and A. Weimer, "Tungsten Nitride ALD Nanofilms for Reducing Hydrogen Diffusion," *American Institute of Chemical Engineers Annual Meeting*, Orlando, Florida, November 2019.
212. Bull, S., T. Champ, R. O'Brien, C. Musgrave, and A. Weimer, "Particle ALD of Tungsten Nitride As a Hydrogen Environmental Barrier Coating for Nuclear Space Propulsion," *American Institute of Chemical Engineers Annual Meeting*, Orlando, Florida, November 2019.
213. Hoskins, A., S. Millican, T. Gossett, Y. Gao, Z. Liang, C. Musgrave, and A. Weimer, "Improved Understanding of the Role of Ultra-Thin ALD Films on Lithium Metal Oxide Cathode Materials," *American Institute of Chemical Engineers Annual Meeting*, Orlando, Florida, November 2019.
214. O'Toole, R., C. Bartel, C. Gump, , C. Musgrave, and A. Weimer, "Particle Atomic Layer Deposition of Yttrium Oxide for Hydrolysis Protection and Sintering of Aluminum Nitride Particles," *American Institute of Chemical Engineers Annual Meeting*, Orlando, Florida, November 2019.
215. Bull, S. K., W. McNeary, C. Adkins, T. Champ, C. Hill, R. O'Brien, C. Musgrave, and A. Weimer, "Atomic Layer Deposition of Ultra-High Temperature Ceramics as Hydrogen Environmental Barrier Coatings for Nuclear Thermal Propulsion." *International Conference and Exposition on Advanced Ceramics and Composites*. Daytona Beach, FL, January 2020.
216. Bull, S. K., W. McNeary, C. Adkins, T. Champ, C. Hill, R. O'Brien, C. Musgrave, and A. Weimer, "Particle Atomic Layer Deposition of Tungsten Nitride as a Hydrogen Environmental Barrier Coating." *International Conference and Exposition on Advanced Ceramics and Composites*. Daytona Beach, FL, January 2020.
217. Kim, K; C. Musgrave, and J. Stansbury, "Utilization of Amine-Peroxide Redox Polymerization (APRP): Progress to Athermal Shadow-curing and More", *Fundamentals and Applications of photopolymerization - Industry-University Cooperative Research Center Spring Meeting*, Iowa City, IA, January 2020.

218. O'Toole, R., C. Hill, P. Buur, C. Bartel, C. Gump, C. Musgrave, and A. Weimer, "Particle Atomic Layer Deposition of Yttrium Oxide for Hydrolysis Protection and Sintering of Aluminum Nitride," *44th International Conference and Exposition on Advanced Ceramics and Composites*, Daytona Beach, Florida, January 2020.
219. Bare, Z., R. Morelock, C. Sutton, C. Musgrave, "Structural and Stability Trends in Single (ABO₃) Perovskite Oxides from DFT-Optimized Bond Valence Structures," *American Chemical Society National Meeting*, Boston, MA, August 2021.
220. Singstock, N., C. Musgrave, "Machine Learning Guided Synthesis of Multinary Chevrel Phases for Tunable Energy Materials," *American Chemical Society National Meeting*, Boston, MA, August 2021.
221. Bare, Z., R. Morelock, C. Sutton, C. Musgrave, "Structural and Stability Trends in Single (ABO₃) Perovskite Oxides from DFT-Optimized Bond Valence Structures," *American Institute of Chemical Engineers Annual Meeting*, Boston, MA, November 2021.
222. Singstock, N., C. Musgrave, "Machine Learning Guided Synthesis of Multinary Chevrel Phases for Tunable Energy Materials," *American Institute of Chemical Engineers Annual Meeting*, Boston, MA, November 2021.
223. Morelock, R., Z. Bare, C. Musgrave, "Computationally accelerated discovery of Gd-based perovskite oxides for solar thermochemical applications", *ACS Spring Meeting*, San Diego, CA, March 2022.

Ph.Ds. – GRADUATED

Jeungku Kang, Materials Science and Engineering, Stanford University, January 2002.
 Yuniarto Widjaja, Chemical Engineering, Stanford University, March 2002.
 Scott Centoni, Materials Science and Engineering, Stanford University, November 2002.
 Collin Mui, with Stacey Bent, Chemical Engineering, Stanford University, December 2002.
 Juan Senosiain, Materials Science and Engineering, Stanford University, December 2002.
 Seongjun Park, with Keongjae Cho, Chemical Engineering, Stanford University, March 2003.
 Joseph Han, Chemical Engineering, Stanford University, June 2004.
 Ye Xu, Materials Science and Engineering, Stanford University, 2006.
 Rojana, Pornpratsertsuk, with F. Prinz, Materials Science and Engineering, Stanford University, 2007.
 Paul Zimmerman, Chemical Engineering, Stanford University, May 2010
 Pendar Ardalan, with Stacey Bent, Chemical Engineering, Stanford University, November 2010
 Aaron Holder, Chemistry and Physics, University of Colorado, April 2014
 Ann Deml, with Ryan O'Hare, Materials Science, Colorado School of Mines, July 2014
 Chris Muhich, with A. Weimer, Chemical Engineering, University of Colorado, November 2014
 Jonathan Tebbe, Chemical Engineering, University of Colorado, January 2015
 Matthias Young, with S. George, Chemical Engineering, University of Colorado, April 2015
 Chern-Hooi Lim, Chemical Engineering, University of Colorado, November 2015
 Chris Bartel, with A. Weimer, Chemical Engineering, University of Colorado, October 2018
 Amanda Hoskins, with A. Weimer, Chemical Engineering, University of Colorado, Nov. 2018
 Samantha Miller, with A. Weimer, Chemical Engineering, University of Colorado, April 2019
 Ryan Trottier, Chemical Engineering, University of Colorado, April 2020
 Jacob Clary, with A. Weimer, Chemical Engineering, University of Colorado, April 2020

Kang Min Kim, with J. Stansbury, Chemistry, University of Colorado, August 2020
Rebecca O'Toole, with A. Weimer, Chemical Engineering, Colorado 2021
Sarah Bull, with A. Weimer, Chemical Engineering, Colorado 2021
Nicholas Singstock, Chemical Engineering, Colorado, 2022
Mohammed Alkhater, Chemical Engineering, Colorado, 2022
Alex Jenkins, with W. Medlin, Chemical Engineering, Colorado, 2022
Zachary Bare, Chemical Engineering, Colorado, 2023
Yousef Al Sunni, Chemical Engineering, Colorado, 2023
Aziz Al-Herz, Chemical Engineering, Colorado, 2023
Ryan Moorelock, Chemical Engineering, Colorado, 2023

Ph.Ds. - CURRENT

Yu Zhou, Chemistry, University of Colorado, 2024
Paige Brimley, with W. Smith, Chemical Engineering, Colorado, 2024
Todd Whittaker, with Adam Holewinski, Chemical Engineering, 2025
Suxuen Yew, Chemical Engineering, 2025
Ahmed Biby, Materials Science and Engineering, 2026
Cooper Tezak, Chemical Engineering, 2026
Benjamin Rich, Chemistry, 2026
Sophie Gerits, Chemical Engineering, 2027
Nima Amiri, Mechanical Engineering, 2027
Eva Arm, Chemical Engineering, 2028
Fatma Salem, Chemical Engineering, 2028
Varun Awasthi, Chemical Engineering, 2028

MASTERS STUDENTS SUPERVISED

Michael Mysinger, Chemical Engineering, Stanford University, 2000
Michael Hall, Chemical Engineering, Stanford University, 2000
Guillaume Dupont, Chemical Engineering, Stanford University, 2004
Pierre Maissa, Mechanical Engineering, Stanford University, 2005
Bariz Sudhanshu, Chemical Engineering, Stanford University, 2007
Christopher McCormick, Chemical Engineering, Stanford University, 2006.
Chenyu Wang, Materials Science and Engineering, Stanford University, 2007
Abby Tyler, Chemical Engineering, University of Colorado, 2009.
Sean Ryland, Chemical Engineering, University of Colorado, 2012
Yu-Ching Kuo, Chemical Engineering, University of Colorado, 2015
Philip Lehman, Chemical Engineering, University of Colorado, 2016
Marie Ambruster, Chemical Engineering, University of Colorado, 2021
Hussain Almajed, Chemical Engineering, University of Colorado, 2021

UNDERGRADUATE RESEARCH and HONORS THESIS SUPERVISED

Alan Derk, University of Colorado
Josh Pacheco, University of Colorado
Jay Wescott, University of Colorado
Timothy Morris, University of Colorado

Aziz Alherz, University of Colorado
Treven Hunter, University of Colorado
Sam Bacon, University of Colorado
Emily Fischer, University of Colorado
Thomas Fuerst, University of Colorado
Hassam Hasoon, University of Colorado
Afnan Alghannam, University of Colorado
Phil Siegel, University of Colorado
Jay Saunders, University of Colorado
Marc Thompson, University of Colorado
Matthew Jankoski, University of Colorado
Charles Musgrave III, University of Colorado

POSTDOCTORAL FELLOWS SUPERVISED

Alessandra Ricca, 1997-1998
Collin Mui, 2003-2004
Atashi Mukhopadhyay, 2005-2007
Gang Zhang, 2005-2006
Ankan Paul, 2005-2007
Blanka Magyari-Kope, with Yoshio Nishi, 2006-2007
Christopher Bartel, 2018-2019
Samantha Millican, 2019-2020
Nicholas Singstock, 2022-
Ryan Morelock, 2023-

COURSES TAUGHT

Stanford University

Solid-State Thermodynamics (Graduate), Department of Materials Science and Engineering, 1996-2003

Quantum Simulations of Molecules and Materials (Graduate), Department of Chemical Engineering, 2000-2003, 2005-2007

Chemical Separations (Undergraduate), Department of Chemical Engineering, 1997-2007

Statistical Mechanics (Graduate), Department of Chemical Engineering, 2005-2006

Harvard University

Physical Chemistry: Quantum Mechanics (Undergraduate), Department of Chemistry and Chemical Biology, 2004

University of Colorado

Introduction to Quantum Simulations, (Undergraduate and Graduate), Department of Chemical and Biological Engineering, 2008, 2010, 2015

Chemical Engineering Reaction Kinetics, (Undergraduate), Department of Chemical and Biological Engineering, 2009, 2010, 2011

Energy Fundamentals, (Undergraduate), Department of Chemical and Biological Engineering, 2009, 2010, 2011, 2013, 2017

Chemistry for Engineers, (Undergraduate), Department of Chemical and Biological Engineering, 2012, 2013.

Physical Chemistry for Engineers, (Undergraduate), Department of Chemical and Biological Engineering, 2014, 2015, 2016

Chemical Separations, (Undergraduate), Department of Chemical and Biological Engineering, 2019

COURSE SURVEYS: INSTRUCTOR RATINGS FOR COURSES TAUGHT

Stanford and Harvard ratings are on a scale of 1 to 5, with 1 being excellent and 5 being poor. University of Colorado ratings are on a 1 to 6 scale with 6 being best. Percentiles signify percentage of instructors receiving a lower Instructor Rating for the quarter.

Course	Term Taught	Enrolled	Responses	Instructor Rating*	School Rating*	%
MSE 202 (G Units 3) Solid State Thermodynamics	Autumn 96-97	30	29	3.00	1.86	3
MSE 202 (G Units 3) Solid State Thermodynamics	Autumn 97-98	37	35	2.44	1.88	12
ChE 120 (UG Units 3) Separation Processes	Spring 97-98	19	16	2.06	1.80	26
MSE 202 (G Units 3) Solid State Thermodynamics	Autumn 98-99	52	45	2.44	1.86	16
ChE 120 (UG Units 3) Separation Processes	Spring 98-99	13	10	1.30	1.77	86
MSE 192/202 (G Units 3) Solid State Thermodynamics	Autumn 99-00	46	39	1.72	1.87	48
ChE 444A (G Units 3) Quantum Simulations Molecules & Materials	Winter 99-00	18	16	1.25	1.83	90
ChE 130 (UG Units 3) Separation Processes	Spring 99-00	18	16	1.25	1.78	87
MSE 202 (G Units 3) Solid State Thermodynamics	Autumn 00-01	28	24	1.96	1.76	27
ChE 444A (G Units 3) Quantum Simulations Molecules & Materials	Winter 00-01	13	12	1.08	1.77	96
ChE 130 (UG Units 3) Separation Processes	Spring 00-01	20	13	1.23	1.73	90

MSE 202 (G Units 3) Solid State Thermodynamics	Autumn 01-02	29	28	1.93	1.75	27
ChE 444A (G Units 3) Quantum Simulations Molecules & Materials	Winter 01-02	22	21	1.00	1.73	100
ChE 130 (UG Units 3) Separation Processes	Spring 01-02	32	30	1.33	1.77	78
MSE 202 (G Units 3) Solid State Thermodynamics	Autumn 02-03	24	21	2.42	1.77	19
ChE 444A (G Units 3) Quantum Simulations Molecules & Materials	Winter 02-03	13	12	1.25	1.65	84
ChE 130 (UG Units 3) Separation Processes	Spring 02-03	24	27	1.31	1.75	76
ChE 444A (G Units 3) Quantum Simulations Molecules & Materials	Winter 04-05	25	20	1.24	1.70	89
ChE 130 (UG Units 3) Separation Processes	Spring 04-05	27	25	1.48	1.72	64
ChE 430 (G Units 3) Statistical Mechanics	Autumn 05-06	50	50	2.3	N/A	N/A
ChE 444A (G Units 3) Quantum Simulations Molecules & Materials	Winter 05-06	40	25	1.2	N/A	N/A
ChE 130 (UG Units 3) Separation Processes	Spring 05-06	14	13	1.2	N/A	N/A
ChE 430 (G Units 3) Statistical Mechanics	Autumn 06-07	27	25	1.6	N/A	N/A

**Course Survey: Instructor Rating for Quantum Chemistry (Harvard University –
Converted from 1 to 5 scale, 1 is best)**

Chemistry 160 (UG) Quantum Mechanics	Fall 04-05	45	30	1.3	NA	NA
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**Course Survey: Instructor Rating for Introduction to Quantum Simulations (University of
Colorado – 1 to 6 scale, 6 being best)**

Course	Term Taught	Enrolled	Responses	Instructor Rating*	Course Rating	%
CHEN 4838/5838 (UG/G) Quantum Simulations	Fall 08-09	17	14	5.9	5.6	99
CHEN 4330 (UG) Chemical Engineering Kinetics	Spring 08-09	49	44	5.3	4.7	68
CHEN 4838 Energy Fundamentals	Fall 09-10	44	35	5.3	5.0	NA
CHEN 4330 (UG) Chemical Engineering Kinetics	Spring 09-10	47	40	5.0	4.7	NA
CHEN 4838/5838 (UG/G) Quantum Simulations	Fall 10-11	33	26	5.5	5.2	NA
CHEN 4838 (UG) Energy Fundamentals	Fall 10-11	48	36	5.3	4.9	NA
CHEN 4330 (UG) Chemical Engineering Kinetics	Spring 10-11	58	45	3.6	3.8	NA
CHEN 4838 (UG) Energy Fundamentals	Fall 11-12	38	28	5.2	5.1	NA
Course	Quarter Taught	Enrolled	Responses	Instructor Rating*	Course Rating	Percentil e
CHEN 4330 (UG) Chemical Engineering Kinetics	Spring 11-12	41	18	5.7	5.3	NA
CHEN 1211 (UG) Gen. Chemistry for Engineers	Fall 12-13	441	182	3.8	3.9	NA
CHEN 4838 (UG) Energy Fundamentals	Spring 12-13	39	33	5.9	5.6	NA
CHEN 1211 (UG) Gen. Chemistry for Engineers	Fall 13-14	308	163	3.8	3.9	NA

CHEN 4521 (UG) Physical Chemistry for Engineers	Spring 13-14	188	140	3.1	2.8	NA
CHEN 4521 (UG) Physical Chemistry for Engineers	Spring 14-15	106	80	4.9	4.2	NA
CHEN 4521 (UG) Physical Chemistry for Engineers	Spring 14-15	98	82	3.9	3.5	NA
CHEN 5838 (G) Quantum Simulations	Fall 15-16	30	25	5.4	4.7	NA
CHEN 4521 (UG) Physical Chemistry for Engineers	Spring 15-16	91	78	4.6	4.2	NA
CHEN 4521 (UG) Physical Chemistry for Engineers	Spring 15-16	96	78	4.5	4.0	NA