Charles Bruce Musgrave

## Chair and Professor of Chemical and Biochemical Engineering

*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

2016 – Chair of Chemical and Biological Engineering

 University of Colorado Boulder, Boulder, CO

2016 – 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

2004 – 2005 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

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

1989 Ford Foundation Fellowship

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

**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).
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).
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).
5. Ricca, A. and C. Musgrave, "Theoretical Study of the Cl-Passivated Si (111) Surface," *Surface Science* 430, 116-125 (1999).
6. Wang, G., C. Mui, C. Musgrave and S. Bent, "Cycloaddition of Cyclopentadiene and Dicyclopentadiene on Si (100)-2x1: Comparison of Monomer and Dimer Adsorption," *Journal of Physical Chemistry B* 102, 6803-6808 (1999).
7. Widjaja, Y., M. Mysinger and C. Musgrave, "An Ab Initio Study of Adsorption and Decomposition of NH3 on Si (100)-2x1," *Journal of Physical Chemistry B* 104, 2527-2533 (2000).
8. Mui, C., S. Bent and C. Musgrave, "A Theoretical Study of the Structure and Thermochemistry of 1,3-butadience on the Ge/Si (100)-2x1 Surface," *Journal of Physical Chemistry A* 104, 2457-2462 (2000).
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).
10. Widjaja, Y. and C. Musgrave, "A DFT Study of Nonlocal Effects on NH3 Adsorption and Dissociation on Si (100)-2x1," *Surface Science* 469, 9-20 (2000).
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).
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).
13. Wang, G., C. Mui, C. Musgrave, and S. Bent, "Effect of a Methyl-Protecting Group on the Adsorption of Pyrrolidine on Si (100)-2x1," *Journal Physical Chemistry B* 105, 3295-3299 (2001).
14. Mui, C., G. Wang, S. Bent, and C. Musgrave, "Reactions of Methylamines at the Si(100)-2x1 Surface," *Journal of Chemical Physics* 114, 10170-10180 (2001).
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)-2x1 Using NH3,” *Physical Review B* 64, 205303-205312 (2001).
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).
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).
19. Wang, G., C. Mui, C. Musgrave, and S. Bent, "Example of a Thermodynamically Controlled Reaction on a Semiconductor Surface: Acetone on Ge (100)-2x1," *Journal of Physical Chemistry B* 105, 12559-12565 (2001).
20. Lee, S., C. Musgrave, P. Zhao, and J. Stebbins, "Topological Disorder and Reactivity of Borosilicate Glasses: Quantum Chemical Calculations and 12O and 11B NMR Study," *Journal of Physical Chemistry B* 105, 12583-12595 (2001).
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). http://dx.doi.org/10.1063/1.1415079
22. Kang, J. and C. Musgrave, "The Mechanism of HF/H2O Chemical Etching of SiO2," *Journal of Chemical Physics* 116, 275-280 (2002).
23. Kang, J. and C. Musgrave, "The Mechanism of Atomic Layer Deposition of SiO2 on the Silicon (100)-2x1 Surface Using SiCl4 and H2O as Precursors," *Journal of Applied Physics* 91, 3408-3414 (2002).
24. Widjaja, Y. and C. Musgrave, "A DFT Study of Atomic Nitrogen on the Si(100)-(2x1) Surface," *Journal Physical Chemistry B* 106, 2643-2648 (2002).
25. Widjaja, Y. and C. Musgrave, "Atomistic Mechanism of the Initial Oxidation of the Clean Si (100)-2x1 Surface by O2 and SiO2 Decomposition," *Journal of Chemical Physics* 116, 5774-5780 (2002).
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](http://dx.doi.org/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) 2x1 Surface," *Journal of Chemical Physics* 116, 9907-9913 (2002).
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)-2x1 and Ge (100)-2x1," *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)-2x1,” *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)-2x1," *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 NH2 + CH4 → NH3 + CH3 and Comparison with Transition State Theory,” *International Journal of Chemical Kinetics* 35, 304-309 (2003). DOI: 10.1002/kin.10131
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39. Widjaja, Y. and C. Musgrave, "Indirect Adsorbate-Adsorbate Interactions Mediated Through the Surface Electronic Structure of the Si (100)-(2x1) Surface," *Journal of Chemical Physics* 120, 1555-1559 (2004). DOI: [10.1063/1.1631932](http://adsabs.harvard.edu/cgi-bin/nph-abs_connect?fforward=http://dx.doi.org/10.1063/1.1631932)
40. Han, J., G. Gao, Y. Widjaja, E. Garfunkel, and C. Musgrave, “A Quantum Chemical Study of ZrO2 Atomic Layer Deposition Growth Reactions on the SiO2 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 Al2O3 Atomic Layer Deposition on SAMs: Effect of SAM Termination,” *Chemistry of Materials,* 16, 646-653 (2004). DOI: 10.1021/cm035009p
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43. Heyman, A. and C. Musgrave, “A Quantum Chemical Study of Atomic Layer Deposition of Al2O3 Using AlCl3 and H2O 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
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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
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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
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63. Mukhopadhyay, A., J. Sanz and C. Musgrave, “First-Principles Investigation of Hydroxylated Monoclinic HfO2 Surfaces,” *Chemistry of Materials,* 18, 3397-3403 (2006). DOI: 10.1021/cm060679r
64. Paul, A. and C. Musgrave, “A Detailed Theoretical Study of the Mechanism and Energetics of Methane to Methanol Conversion by Cis-Platin and Catalytica,” *Organometallics*, 26, 793-809 (2007). DOI: 10.1021/om060465j
65. Huang, K., J. Han, C. Musgrave, and E. Fujita,“Carbon Dioxide Reduction by Pincer Rhodium ŋ2-Dihydrogen Complexes: Hydrogen Binding Modes and Mechanistic Studies by Density Functional Theory Calculations,” *Organometallics,* 26, 508-513, (2007). DOI: 10.1021/om060797o
66. Filler, M., C. Musgrave and S. Bent, “Carbon-Oxygen Coupling in the Reaction of Formaldehyde on Ge (100)−2×1,” *Journal of Physical Chemistry C*, 111, 1739-1746 (2007). DOI: 10.1021/jp064820v
67. Zhang, G. and C. Musgrave, “Comparison of DFT Methods for Molecular Orbital Eigenvalue Calculations,” *Journal of Physical Chemistry A*, 111, 1554-1561 (2007). DOI: 10.1021/jp061633o
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84. Pelz, K., C. Musgrave, J. Falconer and J. Medlin, *“*Effects of Water and Formic Acid Adsorption on the Electronic Structure of Anatase TiO2 (101),” *Journal of Physical Chemistry C*, 115 (6), 2738-2749 (2011). DOI: 10.1021/jp109014a
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100. Lim, C., A. Holder, J. Hynes and C. Musgrave, “Reduction of CO2 to Methanol Catalyzed by a Biomimetic Organo-hydride Produced from Pyridine” *Journal of the American Chemical Society,* 136 (45), 16081-16095 (2014)*.* DOI: 10.1021/ja510131a
101. Deml, A., V. Stevanovic , M. Sanders, A. Holder, C. Musgrave and R. O’Hayre, “Tunable energetics of oxygen vacancy formation in the complex perovskite oxide Sr*x*La1-*x*Mn*y*Al1-*y*O3 (SLMA),” *Chemistry of Materials,* 26 (22), 6595-6602 (2014). DOI: 10.1021/cm5033755
102. Muhich, C., J. Westcott III, T. Fuerst, B. Erhardt, A. Weimer and C. Musgrave, “Increasing Photocatalytic Activity of Anatase TiO2 Through Non-Metal Doping,” *Journal of Physical Chemistry C,* 118 (47), 27415-27427(2014).DOI: 10.1021/jp508882m
103. Muhich, C.L., K.C. Weston, D. Arifin, A.H. McDaniel, C.B. Musgrave, A.W. Weimer. “Extracting Kinetic Information from Complex Gas-solid Reaction Data”, *Industrial and Engineering Chemistry Research,* 54 (16), 4113-4122 (2015). DOI: 10.1021/ie503894f
104. Deml, A.M., A.M. Holder, R.P. O’Hayre, C.B. Musgrave and V. Stevanovic, “Intrinsic Material Properties Dictating Oxygen Vacancy Formation Energetics in Metal Oxides,” *Journal of Physical Chemistry Letters*, 6 (10), 1948-1953 (2015). DOI: 10.1021/acs.jpclett.5b00710
105. Guan, L., M. Li, X. Li, L. Feng, F. Teng, B Liu and C. Musgrave, “Electronic and Dielectric Properties of Ruddlesden-Popper Type and Magnéli Type SrTiO3”, *Computational Materials Science*, 96 Part A, 223-228, (2015). DOI: 10.1016/j.commatsci.2014.09.026
106. Young, M.J., A. M. Holder, S.M. George, and C.B. Musgrave, “Charge Storage in Cation Incorporated a-MnO2,” *Chemistry of Materials*, 27 (4), 1172-1180 (2015). DOI:10.1021/cm503544e
107. Young, M.J., C.B. Musgrave and S.M. George, “Growth and Characterization of Al2O3 Atomic Layer Deposition Films on sp2-Graphitic Carbon Substrates Using NO2/Trimethylaluminum Pretreatment,” *ACS Applied Materials and Interfaces*, 7 (22), 12030-12037 (2015). DOI: 10.1021/acsami.5b02167
108. Muhich,C.L., J. Qiu, A.M. Holder, Y.C. Wu, A.W. Weimer, W.D. Wei, L. McElwee-White, and C.B. Musgrave, “Solvent Control of Surface Plasmon Mediated Chemical Deposition of Au Nanoparticles from Alkylgold Phosphine Complexes”, *ACS Applied Materials and Interfaces*, 7 (24), 13384-13394 (2015). DOI: 10.1021/acsami.5b01918
109. Tebbe, J., T. Fuerst, and C.B. Musgrave, “Mechanism of hydrofluoric acid formation in ethylene carbonate electrolytes with fluorine salt additives,” *Journal of Power Sources,* 297 427-435 (2015). DOI: 10.1016/j.jpowsour.2015.07.104
110. Young, M.J., M. Neuber, A.C. Cavanagh, H. Sun, C.B. Musgrave, and S.M. George, “Sodium Charge Storage in Thin Films of MnO2 Derived by Electrochemical Oxidation of MnO Atomic Layer Deposition Films**,**” *Journal of the Electrochemical Society*, 162 (14), A2753=A2761 (2015). DOI: 10.1149/2.0671514jes
111. Tebbe, J., A.M. Holder, and C.B. Musgrave, “Mechanisms of LiCoO2 Cathode Degradation by Reaction with HF and Protection by Thin Oxide Coatings,” *ACS Applied Materials and Interfaces,* 7 (43). 24265-24278 (2015). DOI: 10.1021/acsami.5b07887
112. Lim, C.H., A.M. Holder, J.T. Hynes, and C.B. Musgrave, “Renewable Organo Hydrides for Catalytic Reduction of CO2 to Fuels,” *Journal of Physical Chemistry Letters*, 6 (24), 5078-5092 (2015). DOI: 10.1021/acs.jpclett.5b01827
113. Muhich, C.L., B. Ehrhart, V. Witte, S.L. Miller, E. Coker, C.B. Musgrave, A.W. Weimer, “Predicting the Solar Thermochemical Water Splitting Ability and Reaction Mechanism of Metal Oxides: A Case Study of the Hercynite Family of Water Splitting Cycles”, *Energy and Environmental Science*, 8, 3687-3699 (2015). DOI: 10.1039/C5EE01979F
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127. Alherz, A., C-H. Lim, J. T. Hynes, and C.B. Musgrave\*, “Predicting Hydride Donor Strength Via Quantum Chemical Calculations of Hydride Transfer Activation Free Energy,” *Journal of Physical Chemistry B,* 122 (3), 1278-1288 (2018). DOI:10.1021/acs.jpcb.7b12093
128. Hoskins, A., A. Coffey, C. Musgrave and A.W. Weimer\*, “Nanostructured Mullite Oxidation Resistant Coatings for SiC Developed via Atomic Layer Deposition,” *J. Amer. Ceram. Soc.*, 101 (6) 2493-2505 (2018). DOI:10.1111/jace.15408
129. Ilic, S. A. Alherz, C.B. Musgrave, K.D. Glusac\*, “Thermodynamic and Kinetic Hydricities of Metal-Free Hydrides,” *Chemical Society Reviews*, 47, 2809-2836 (2018). [DOI: 10.1039/C7CS00171A](http://dx.doi.org/10.1039/C7CS00171A)
130. Love, D., K. M. Kim, C.B. Musgrave, C.N. Bowman\*, “Amine Induced Retardation of the Radical-Mediated Thiol-Ene Reaction via the Formation of Metastable Disulfide Radical Anions,” *Journal of Organic Chemistry*, 83 (5), 2912-2919 (2018). DOI:10.1021/acs.joc.8b00143
131. Stevanovic\*, V., R. Trottier, C. Musgrave, F. Therrien, A. Holder and P. Graf, “Efficient Assessment of Kinetics of Polymorph Transformations,” *Physical Review Materials,* 2 (3),033802 (2018). DOI:10.1103/PhysRevMaterials.2.033802
132. Talley, K., S.M. Millican, A.M. Holder, C.B. Musgrave, J. Mangum, G. Brennecka, S. Siol, A. Zakutayev, “Understanding the Aluminum-Scandium Nitride Heterostructural Alloy System Through Computation and Combinatorial Synthesis,” *Physical Review Materials,* 2 (6), 063802 (2018). DOI:10.1103/PhysRevMaterials.2.063802
133. Worrell, B., M. McBride, G. Lyon, L. Cox, C. Wang, S. Mavilla, C-H. Lim, H. Coley, C. Musgrave, Y. Ding and C. Bowman, “Bistable and Photoswitchable States of Matter,” *Nature Communications*, 9, (2018). [DOI: 10.1038/s41467-018-05300-7](https://doi.org/10.1038/s41467-018-05300-7)
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136. Bartel, C.J., S.L. Millican, A.M. Deml, J.R. Rumptz,W. Tumas, A.W. Weimer, S. Lany, V. Stevanovic, C. B. Musgrave,\* and A.M. Holder\*, “Machine Learning The Gibbs Energy of Inorganic Crystalline Solids,” *Nature Communications*, 9 (2018). DOI: [10.1038/s41467-018-06682-4](https://doi.org/10.1038/s41467-018-06682-4)
137. Alherz, A., P. Lehman, Y. Kuo, C-H. Lim, A. Holder, J. Hynes, J. Cha and C. Musgrave, “Renewable Hydride Donors for the Catalytic Reduction of CO2: A Thermodynamic and Kinetic Study”, *Journal Physical Chemistry B*., (2018). DOI: 10.1021/acs.jpcb.8b08536
138. Mavila, S., B. Worrell, H. Culver, T. Goldman, C. Wang, C-H Lim, D. Domaille, S. Pattanayak, M. McBride, C. Musgrave and C. Bowman, “Dynamic and Responsive DNA-Like Polymers,” *Journal of the American Chemical Society* 140, 13594-135-98 (2018). DOI:10.1021/jacs.8b09105
139. Bartel, C., V. Stevanovic, C. Musgrave, A. Holder, “Considerations for High-throughput Predictions of Solid Stability Using Density Functional Theory,” *npj Computational Materials,* 5 (1), 4 (2019).DOI: 10.1038/s41524-018-0143-2
140. Lim, C., S. Ilic, A. Alherz, B. Worrell, S. Bacon, J. Hynes, K. Glusac and C. Musgrave, “Benzimidazoles as Metal-Free and Renewable Hydrides for CO2 Reduction to Formate,” *Journal of the American Chemical Society*, 141 (1), 272-280 (2019). DOI: 10.1021/jacs.8b09653
141. O’Toole, R., C. Bartela, M. Kodasa, A. Horrella, S. Ricote, N. Sullivan, R. Hall, C. Musgrave and A. Weimer, “Particle Atomic Layer Deposition of Alumina for Sintering Yttria-stabilized Cubic Zirconia,” *Journal of the American Ceramic Society*, In Press (2019). DOI: [doi.org/10.1111/jace.16091](https://doi.org/10.1111/jace.16091)
142. Hoskins, A., T. Gossett, C. Musgrave and A. Weimer, “The Effect of Ultrathin ALD Films on the Oxidation Kinetics of SiC in High-Temperature Steam,” *Journal of the American Ceramic Society,* In press (2019).
143. Bartel, C.J., C. Sutton, B.R. Goldsmith, R. Ouyang, C.B. Musgrave, L.M. Ghiringhelli, M. Scheffler, “New Tolerance Factor to Predict Perovskite Oxide and Halide Stability,” *Science Advances,* In press (2019).

**ARTICLES UNDER REVIEW**

1. Han, Y., R. Trottier, S. Siol, B. Matthews, M. Young, C. Musgrave, S. Lany, J. Tate, Q. Zhang, A. Holder, A. Zakutayev, “Epitaxial Templating of Wurtzite MnTe on ZnTe Seed Layer,” J. of Phys. Chem. Lett., Submitted, August 2018.
2. Millican, S., A. Hoskins, C. Czernik, I. Alshakiti, J. Netter, C. Musgrave and A. Weimer, “On-Sun Demonstration of Redox Driven Solar Thermochemical Hydrogen Production,”, *Applied Energy*, Submitted, October 2018.
3. Hoskins, A., T. Gossett, S. Millican, Y. Gao, X. Liang, C. Musgrave and W. Weimer, “Non-Uniform Growth of Ultra-thin ALD Films on Lithium Metal Oxide Materials,” *Nature Communications*, Submitted, November 2018.
4. Kim, K. N. Singstock, K. Childress, J. Sinha, A. Salazar, S. Whitfield, A. Holder, J. Stansbury and C. Musgrave, “Rational Design of Efficient Amine Redox Initiators for Amine-Peroxide Redox Polymerization”, Journal of the American Chemical Society, Submitted, December 2018.
5. Bartel, C., C. Sutton, B. Goldsmith, A. Holder and C. Musgrave, “Prediction of Stable Double Perovskite Halides as Efficient Solar Absorbers,” Submitted, December 2018.
6. Bartel, C., J. Rumptz, A. Holder, A. Weimer and C. Musgrave, “High-throughput Equilibrium Analysis of Active Materials for Solar Thermochemical Ammonia Synthesis,” Submitted December 2018.
7. Clary, J., S. Van Norman, H. Funke, C. Majlinger, D. Su, E. Stach, J. Falconer, C. Musgrave and A. Weimer, “Highly Dispersed Co Metal Deposited via Thermal Cp/H2 Particle Atomic Layer Deposition,” Submitted, December 2018.

**INVITED NON-PEER REVIEWED ARTICLES**

1. Musgrave, C., Stanford University, Lux Capital Nanotechnology Report, 2001.
2. Musgrave, C., Stanford University, Lux Capital Nanotechnology Report, 2004.
3. Musgrave, C. and R. Gordon, “Precursors for Atomic Layer Deposition of High-K Dielectrics,” FutureFab International, 18, January 2005.

**ARTICLES IN CONFERENCE PROCEEDINGS**

1. Zubkov, V., J. Senosiain, S. Aronowitz, V. Sukharev, and C. Musgrave, “Boron Diffusion Mechanism in Silicon Oxide Using Ab Initio Methods,” *Materials Research Society Symposium* 610, B3.11.1 (2000).
2. Zubkov, V., J. Han, G. Sun, C. Musgrave and S. Aronowitz, “Modeling Copper Diffusion in Silicon Oxide, Nitride and Carbide”, *Materials Research Society Symposium*, 716, B8.4.1 (2002).
3. Gao, G., J. Han, Y. Widjaja, E. Garfunkel, and C. Musgrave, “Quantum Chemical Study of ZrO2 Atomic Layer Deposition on the SiO2 Surface,” *Invited Paper*, *Electrochemical Society International Symposium: Chemical Vapor Deposition XVI and EUROCVD 14* 2003-08, 1-14 (2003).
4. Ardalan, P., C. Musgrave and S. Bent, “Effects of Surface Functionalization on Titanium Dioxide Atomic Layer Deposition on Ge Surfaces,” *Electrochemical Society Transactions*, 25 (4), 131 (2009).
5. Yoon, B., Y. Lee, A. Derk, C. Musgrave and S. George, "Molecular Layer Deposition of Conductive Hybrid Organic-Inorganic Thin Film Polymers using Diethylzinc and Hydroquinone," *Electrochemical Society Transactions*, 33 (27), 191-195 (2011).

BOOK CHAPTER

1. Musgrave, C., “Theoretical Modeling of ALD Processes”, *Atomic Layer Deposition of Nanostructured Materials*, Editors: N. Pinna and M. Knez, Wiley-VCH Verlag & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany, 2012.

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

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

Physical Review B

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

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-

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-

Faculty Search Committees, Department of Chemical and Biological Engineering

Chair Search Committee, Department of Chemical and Biological Engineering

Campus Representative - Colorado Collaborative Research Computing Board, 2011-

Chair - Curriculum Development Committee - Materials Science Program, 2011-

University Executive Advisory Council to the Graduate School, 2011-

Associate Chair, Department of Chemical and Biological Engineering, 2011-

Graduate Program Director, Department of Chemical and Biological Engineering, 2011-

Executive Committee - Materials Science Program, 2012 –

Graduate Admissions Committee - Materials Science Program, 2013 -

FLAG Leadership Committee, College of Engineering 2013 -2014

Strategic Hiring Committee, RASEI, 2014-

Department Chair, Department of Chemical and Biological Engineering, 2016-

###### 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 Système du CNRS, Université Paul Sabatier Toulouse III, Toulouse, France (2006)

Ph.D. Thesis Committee, Phillipe 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, Panel Review, CTS, Solar Energy, December 2007.

Science Foundation Ireland, Nanoscience Research Center Review, Panel Chair, December 2012-January 2013.

##### 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 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 Chairman, 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 Chairman, 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

**CONFERENCE SESSION CHAIRS**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

**INVITED CONFERENCE PRESENTATIONS**

1. Goddard, W., K. Lim, M. Belmares, X. Chen, J. Hu, C. Musgrave, F. Faglioni, J. Perry and D. Lu, “Simulation and Design of Materials – Applications to Polymers, Ceramics, Semiconductors, and Catalysis,” *American Chemical Society National Meeting,* Los Angeles, March 1993.
2. Goddard, W., C. Musgrave, J. Gerdy and J. Perry, “Electronic and Optical Properties for Nanostructures, Monolayers, Superlattices and Clusters,” *American Chemical Society National Meeting,* Chicago, IL, August 1993.
3. Musgrave, C., “Atomic Scale Properties and Engineering of Novel Interfaces: Theory and Simulation,” *American Physical Society*, San Jose, CA, March 1995.
4. Musgrave, C., “Manipulation of Reactivity of Surfaces Using STM for Growing Nanostructures,” *Foresight Conference on Nanotechnology*, Palo Alto, CA, November 1995.
5. Musgrave, C., “The Adsorption and Decomposition of Phosphine on Si(100) 2x1,” *Telluride Workshop on Semiconductor Surface Chemistry*, Telluride, CO, August 1998.
6. Musgrave, C., “Chlorine on Si(111): Non-local Effects on Si-Cl Vibrational Frequencies,” *Telluride Workshop on Semiconductor Surface Chemistry*, Telluride, CO, August 1998.
7. Musgrave, C., “Determining Rate Constants for Surface Reactions for Semiconductor Processing,” *SemiconWest 99*, San Francisco, CA, July 1999.
8. Musgrave, C., “Theoretical Study of Reactions of Ammonia and Phosphine On Si(100) 2x1: Non-local Effects,” *American Chemical Society*, San Francisco, CA, March 2000.
9. D. Golden, J. Senosiain, C. Musgrave, “Use of Ab Initio Quantum Mechanics to Estimate Rate Constants,” *Harold Johnson Festschrift, American Chemical Society*, San Francisco, CA, March 2000.
10. D. Golden, J. Senosiain, C. Musgrave, “Use of Ab Initio Quantum Methods to Estimate Rate Constants,” *Gas Kinetics Conference*, Cambridge, England, July 2000.
11. D. Golden, J. Senosiain, C. Musgrave, “Use of Quantum Methods for a Consistent Approach to Combustion Modeling: Hydrocarbon Bond Dissociation Energies,” *Faraday Discussions*, Leeds University, Leeds, England, July 2001.
12. Senosiain, J., C. Musgrave, D. M. Golden, “Reaction of OH and O (3-PJ) with H2O2: A Comparative Study,” *National Institute of Standards and Technology International Symposium on Kinetics*, Washington, D.C., July 2001.
13. Musgrave, C., “Quantum Chemical Studies of Semiconductor Processing,” *Center for Integrated Systems Annual Advisory Council Meeting*, Stanford University, Stanford, CA, October 2001.
14. Musgrave, C., “Atomic Layer Deposition of High-K Dielectrics,” *Semiconductor Research Corporation Engineering Research Center for Environmentally Benign Semiconductor Processing Teleconference*, January 2002.
15. Musgrave, C., “Selective Atomic Layer Deposition of High-K Dielectrics,” *Semiconductor Research Corporation Engineering Research Center for Environmentally Benign Semiconductor Processing*, University of Arizona, Tucson, AZ, February 2002.
16. Musgrave, C., “Prediction of Schottky Barriers and Contact Resistance of Copper Barrier Layer Interfaces,” *Semiconductor Research Corporation Review*, University of Illinois, Urbana, IL, March 2002.
17. Musgrave, C., “Quantum Chemistry of the Manipulation of Surface Reactions for Nanotechnology,” *American Physical Society*, Cleveland, OH, March 2002.
18. Musgrave, C., “Quantum Chemistry of the Manipulation of Surface Reactions for Nanotechnology,” *American Conference of Theoretical Chemistry*, Seven Springs, PA, July 2002.
19. Musgrave, C., “Quantum Chemical Simulations of Atomic Layer Deposition of High-K Gate Dielectrics,” *Telluride Workshop on Semiconductor Surface Chemistry*, Telluride, CO, August 2002.
20. Musgrave, C., “Germanium Based Integrated Circuits: Atomic Layer Deposition of High-K Dielectrics on Ge,” *Semiconductor Research Corporation Engineering Research Center for Environmentally Benign Semiconductor Processing Teleconference*, October 2002.
21. Musgrave, C., “Simulations of High-K Dielectric Growth by Atomic Layer Deposition,” *Plenary Session:* *American Physical Society*, Austin, TX, March 2003.
22. Musgrave, C., “Computational Prototyping of Nanostructure Fabrication,” *American Chemical Society*, New Orleans, LA, March 2003.
23. Musgrave, C., 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.
24. Musgrave, C., J. Han, Y. Widjaja, “Atomistic Simulations of Atomic Layer Deposition of High-K Dielectrics,” American Vacuum Society; Thin Films User Group, Santa Clara, CA, April 2003.
25. Musgrave, C., “ALD of High-K Dielectrics,” Plenary Talk; *The Annual Electrochemical Society Meeting, Chemical Vapor Deposition XVI/EUROCVD XIV*, Paris, France, April 2003.
26. Musgrave, C., “DFT Simulations of ALD of High-K Thin Films Using Metal Chlorides, Metal Alkyamides, and Alkoxides,” Initiative for Nanoscale Materials Processes, Stanford University, Stanford, CA, July 2003.
27. Musgrave, C., “Chemical Mechanisms of Atomic Layer Deposition of Electronic Materials,” *Gordon Research Conference on the Chemistry of Electronic Materials*, New London, CT, July 2003.
28. Musgrave, C., “Ab Initio Studies of ALD Surface Reactions,” *The Third American Vacuum Society Topical Conference on Atomic Layer Deposition*, San Jose, CA, August 2003.
29. Musgrave, C., “Quantum Chemistry as a Tool for Computational Prototyping of Semiconductor Processes,” *Annual Review NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing*, Stanford, CA, August 2003.
30. Musgrave, C., “Ab Initio Simulations of Atomic Layer Deposition of Metal Oxides,” *American Chemical Society*, New York, NY, September 2003.
31. Musgrave, C., “Theoretical Predictions of the Chemistry of Atomic Layer Deposition,” *NSF Nanoscience Young Scientist Exchange Program,* Massachusetts Institute of Technology, Cambridge, MA, September 2003.
32. Musgrave, C., “DFT Simulations as Engineering Tools for the Computational Prototyping of Nanostructure Fabrication,” *Workshop on Silicon Nanoelectronics and Beyond*, *National Science Foundation National Nanotechnology Initiative,* Portland, OR, October 2003.
33. Musgrave, C., “Modeling and Simulation of Atomic Layer Deposition Chemistry and Kinetics,” *Materials Research Society Advanced Metallization Conference*, Montreal, Canada, October 2003.
34. Musgrave, C., “The Emergence of Nanoscale Technology in Electrical and Chemical Systems”, *The Third Annual Nanotechnology Forum*, Palm Springs, CA, February 2004.
35. Musgrave, C., “The Surface Chemistry of Atomic Layer Deposition,” *2nd Annual UC Surface Science and Applications Symposium,* University of California at San Diego, San Diego, CA, February 2004.
36. Musgrave, C., “Chemistry of Atomic Layer Deposition of High-K Dielectrics: Effect of Substrates and Precursor Selection” *Semiconductor Research Corporation Engineering Research Center for Environmentally Benign Semiconductor Processing Teleconference*, March 2004.
37. Hosack, H., W. Joyner, M. Lundstrom, C. Musgrave, M. Giles, G. Klimeck, V. Varadan, “Mulitiscale, Multiphenomena Modeling and Simulation,” Nanoelectronics and Beyond, NSF-SRC Workshop, Washington, D.C., December 2004.
38. Musgrave, C., “Chemical Mechanisms of the ALD of High-K Dielectrics,” *The Fifth American Vacuum Society Topical Conference on Atomic Layer Deposition*, San Jose, CA, August 2005.
39. Mukhopadhyay, A., Sanz J., and Musgrave, C., “HfO2 Dielectric Surfaces and Interfaces,” *Semiconductor Research Corporation Engineering Research Center for Environmentally Benign Semiconductor Processing Teleconference*, September 2006.
40. Mukhopadhyay, A., Paul, A. and Musgrave, C., “Quantum Simulations of Complex Chemical Processes; Atomic Layer Deposition and Catalysis,” *American Chemical Society Spring Meeting,* Chicago, IL, March 2007.
41. Mukhopadhyay, A., Sanz, J. and Musgrave, C., “Quantum Molecular Dynamics Simulations of the Atomic Layer Deposition of High-K Dielectrics,” *Materials Research Society Spring Meeting,* San Francisco, CA, April 2007.
42. Mukhopadhyay, A., Han, J. and Musgrave, C., “Quantum Simulations of Atomic Layer Deposition of HfO2,” *American Vacuum Society Annual Atomic Layer Deposition Meeting,* San Diego, CA June 2007.
43. Paul, A., Nielsen, L., Jacobsen, E., and Musgrave, C., “Molecular Design of Homogeneous Catalysts for Methane to Methanol Conversion, Enantioselective Epoxide Ring Opening and Other Valuable Transformations,” *American Chemical Society National Meeting,* Boston, MA, August 2007.
44. Mukhopadhyay, A., Sanz, J. and Musgrave, C., “Quantum Simulations of Atomic Layer Deposition of HfO2,” *American Chemical Society National Meeting,* Boston, MA, August 2007.
45. Mukhopadhyay, A., Sanz, J. and Musgrave, C., “Molecular Dynamics Simulations of HfO2 Atomic Layer Deposition,” *American Vacuum Society Annual Meeting,* Seattle, WA 2007.
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 Biomemetic 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., S. Millican, Ryan Trottier, Aaron Holder and C. Bartell, “Ab Initio and Machine Learned Modeling for the Design and Discovery of New Materials for Energy Applications,” *American Chemical Society Spring National Meeting*, Orlando, FL, April 2019.
90. Musgrave, Matthias Young and Aaron Holder, “Unified Band Diagram Framework for the Computational Screening of Ion Intercalation Materials for Next Generation Batteries,” *American Chemical Society Spring National Meeting*, Orlando, FL, April 2019.
91. Musgrave, C., S. Millican, Ryan Trottier, Aaron Holder and C. Bartell, “Ab Initio and Machine Learned Modeling, Design and Discovery of Water Splitting Materials,” *Materials Research Society Spring National Meeting*, Phoenix, AZ, March 2019.

**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-PJ) 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., S. Millican, Aaron Holder and C. Bartell, “Ab Initio and Machine Learned Modeling for the Design and Discovery of New Materials for Energy Applications,” *The Ohio State University*, Columbus, OH, January 2019.

**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 Alkyamides,” 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,” Novelus 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,” Aixstron-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 Six-1Gex 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 Hf(N(CH3)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 HfO2 Using Hafnium Alkylamide Precursors,” *The Fourth American Vacuum Society Topical Conference on Atomic Layer Deposition*, Helsinki, Finland, August 2004.
38. Han, J., S. Wang, R. Gordon and C. Musgrave, “Kinetics of HfO2 ALD Using Hf Chloride and Hf Alkylamide and Water as Precursors,” *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.
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 Hf(N(CH3)2)4 on the SiO2 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.
42. Mui, C., Y. Widjaja, J. Kang and C. Musgrave, “Surface Reaction Mechanisms for CVD and ALD of Silicon Nitride,” *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.
43. Musgrave, C., “Teaching Quantum Chemical Simulations to Chemical Engineers,” *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.
44. Han, J., M. Kelly, G. Parsons and C. Musgrave, “DFT Study of the Initial ALD Reactions of Hf(N(CH3)2)4 on the Si-H Surface: Chemical Mechanism and Vibrational Spectra,” *American Vacuum Society Annual Meeting*, Anaheim, CA, November 2004.
45. Han, J., M. Kelly, G. Parsons and C. Musgrave, “DFT Study of the Initial ALD Reactions of Hf(N(CH3)2)4 on the SiO2 and Si-H Surfaces: Mechanism, Kinetics, Vibrational Spectra and Interface Structure,” *American Vacuum Society Annual Meeting*, Anaheim, CA, November 2004.
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 HfO2,” *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.
51. Mukhopadhyay, A., J. Han and C. Musgrave, “Chemical Mechanisms of Contamination in Atomic Layer Deposition of HfO2,” *American Institute of Chemical Engineers Annual Meeting*, Cincinnati, OH, November 2005.
52. Dupont, G. and and C. Musgrave, “Organic Functionalization of Semiconductors Using Amino Acids: Quantum Resonance Coupling,” *American Institute of Chemical Engineers Annual Meeting*, Cincinnati, OH, November 2005.
53. Mukhopadhyay, A., J. Sanz and C. Musgrave, “Quantum Simulations of Atomic Layer Deposition of HfO2,” *The Electrochemical Society Annual Meeting*, Denver, CO, May 2006.
54. Mukhopadhyay, A., J. Sanz and C. Musgrave, “Ab Initio Phase Diagrams for Water Adsorbed on Monoclinic HfO2,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
55. Dupont, G., P. Ardalan, 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 RuO2 on HfO2 Interfaces,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
57. Mukhopadhyay, A., J. Sanz and C. Musgrave, “Quantum Molecular Dynamics Simulations of the ALD of HfO2,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
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](http://aiche.confex.com/aiche/2006/preliminaryprogram/abstract_76062.htm),” *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.
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166. Miller, S., R. Trottier, K. Sun, A. Weimer and C. Musgrave “Evaluating the Effect of Modeling Variables and Experimental Conditions on Material Development for Solar Thermochemical Water Splitting,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November, 2016.
167. Hoskins, A., A. Coffery, C. Musgrave and A. Weimer, “Stabilizing SiC for Solar Thermal Water Splitting Applications,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November, 2016.
168. Bartel, C., A. Deml, S. Miller, J. Rumptz, A. Weimer, S. Lany, C. Musgrave, V. Stevanovic, and A. Holder, “High-Throughput Prediction of Finite Temperature Compound Gibbs Formation Energies”, *Materials Research Society Fall Meeting*, Boston, MA, December 2016.
169. Hoskins, A., A. Coffey, C. Musgrave and A. Weimer, “Nano-Structured Ceramic Coatings to Stabilize SiC Against Reaction in High Temperature Steam,” 41st *International Conference and Exposition on Advanced Ceramics and Coatings*, Daytona Beach, FL, January, 2017.
170. Millican, S., R. Trottier, K. Sun, A. Weimer, and C. Musgrave “Finite Temperature Modeling of Metal Oxides for Solar Thermochemical Water Splitting,” *American Chemical Society Spring Meeting,* San Francisco, CA, April, 2017.
171. Bartel, C. J., Muhich, C.L., Weimer, A.W., and C.B. Musgrave, “Aluminum nitride hydrolysis enabled by hydroxyl-mediated surface proton hopping,” *American Chemical Society Spring Meeting,* San Francisco, CA, April, 2017.
172. Bartel, C. J., Deml, A. M., Miller, S.L., Rumptz, J.R., Weimer, A.W., Lany, S., Musgrave, C. B., Stevanovic, V., Holder, A. M., “Gibbs energies of solid through materials informatics” *American Chemical Society Spring Meeting,* San Francisco, CA, April, 2017.
173. Millican, S. K. Talley, A. Weimber, C. Musgrave, V. Stevanovic, A. Holder, S. Lany, A. Zakutayev, “Design Principles and Non-Equilibrium Synthesis of Piezoelectric Heterostructural Alloys,” *American Chemical Society Spring Meeting,* San Francisco, CA, April, 2017.
174. Love, D., K. M. Kim, J. Goodrich, B. Fairbanks, W. Xi, B. Worrell, S. Pattanayak, Mark Stoykovich, C. B. Musgrave, C. N Bowman, “Heterofunctional thiol-ene polymerizations for the synthesis of sequence-ordered, biomimetic polymers,” *American Chemical Society Spring Meeting,* Washington D.C., August, 2017.
175. Bartel,C., A. M. Deml, S. L. Millican, J. R. Rumptz, W. Tumas, A. W. Weimer, S. Lany, V. Stevanovic, C. B. Musgrave and A. M. Holder, “[Machine Learning the Thermochemistry of All Inorganic Crystalline Solids](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/496458),” *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November, 2017.
176. Love, D., B. *D. Fairbanks, K. M. Kim, B. Worrell, W. Xi, J. T. Goodrich, C. B. Musgrave, M. Stoykovich and C. N. Bowman*, “[*Hybrid Chain-Growth/Step-Growth Mechanism Observed in Heterofunctional Thiol-Ene Polymerizations*](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/498026),” *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November, 2017.
177. Hoskins, A., A. Coffey, C. B. Musgrave and A. W. Weimer, [“Nano-Structured Ceramic ALD Coatings to Stabilize SiC Against Reaction in High Temperature Steam](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/492741),” *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November, 2017.
178. Millican, S. L., K. Talley, A. W. Weimer, A. Zakutayev, C. B. Musgrave, G. Brennecka and A. Holder, “[Leveraging Heterostructural Alloying to Design Metastable Nitrides with Improved Piezoelectric Properties](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/493051),” *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November, 2017.
179. Love, D., K.M. Kim, J. Goodrich, B. D. Fairbanks, M. Stoykovich, C. B. Musgrave and C. N. Bowman, “[Amine Effects on Radial-Mediated Thiol-Ene Reactions](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/496928),” *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November, 2017.
180. Hoskins, A., A. Coffey, C. B. Musgrave and A. W. Weimer, [“Computational Screening of High Temperature Materials for Environmental Barrier Thin Films](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/492745),” *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November, 2017.
181. Hoskins, A., S. L. Millican, C. Czernik, M. Wallace, I. Al-Shankiti1, J. Netter, C. B. Musgrave and A. W. Weimer, “[Near-Isothermal on-Sun Demonstration to Split Water](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/492700),” *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](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/496428),” *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](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/500399),” *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](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/492988),” *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)](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/496365),” *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November, 2017.
186. Bartel, C. J., J. R. Rumptz, 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](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/496514),” *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](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/500149),” *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November, 2017.
188. Millican, S. L., K. Sun, I. Androshchuk, A. W. Weimer and C. B. Musgrave, [“Assessing the Thermodynamic Viability of Mixed Metal Oxides for Solar Thermochemical Water Splitting](https://aiche.confex.com/aiche/2017/meetingapp.cgi/Paper/Paper/493008),” *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November, 2017.
189. 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.
190. Millican, S., I. Androshchuk, 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.
191. Hoskins, T. Gossett, C. Musgrave and A. Weimer, “Nano-Structured Ceramic ALD Coatings to Stabilitze SiC Against Oxidation in High-Temperature Steam Solar Thermal Water Splitting Applications,” *American Institute of Chemical Engineers Annual Meeting*, Pittsburgh, PA, October, 2018.
192. 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.
193. 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.

**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 Fritz 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 Alan Weimer, Chemical Engineering, University of Colorado, November, 2014

Jonathan Tebbe, Chemical Engineering, University of Colorado, January, 2015

Matthias Young, with Steven George, Chemical Engineering, University of Colorado, April, 2015

Chern-Hooi Lim, Chemical Engineering, University of Colorado, November, 2015

Chris Bartel, Chemical Engineering, University of Colorado, October, 2018

Amanda Hoskins, Chemical Engineering, University of Colorado, November, 2018

**Ph.Ds. - CURRENT**

Ryan Trottier, Chemical Engineering, University of Colorado, 2018

Samantha Miller, Chemical Engineering, University of Colorado, 2018

Jacob Clary, Chemical Engineering, University of Colorado, 2018

Kang Min Kim, Chemistry, University of Colorado, 2019

Yu Zhou, Chemistry, University of Colorado, 2020

Aziz Al-Herz, Chemical Engineering, Colorado, 2020

Rebecca O’Toole, Chemical Engineering, Colorado 2021

Sarah Bull, Chemical Engineering, Colorado 2021

Alex Jenkins, Chemical Engineering, Colorado, 2021

Zachary Bare, Chemical Engineering, Colorado, 2021

Nicholas Singstock, Chemical Engineering, Colorado, 2022

Ryan Moorelock, Chemical Engineering, Colorado, 2023

Mohammed Alkhater, Chemical Engineering, Colorado, 2023

Yousef Al Sunni, Chemical Engineering, Colorado, 2023

Minyan Wang, Materials Science and Engineering, Colorado, 2023

**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, Stanford University, 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

**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

**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

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

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 StateThermodynamics | Autumn96-97 |  30 | 29 | **3.00** | 1.86 | 3 |
| MSE 202 (G Units 3)Solid StateThermodynamics | Autumn97-98 | 37 | 35 | **2.44** | 1.88 | 12 |
| ChE 120 (UG Units 3)Separation Processes | Spring97-98 | 19 | 16 | **2.06** | 1.80 | 26 |
| MSE 202 (G Units 3)Solid StateThermodynamics | Autumn98-99 |  52 | 45 | **2.44** | 1.86 | 16 |
| ChE 120 (UG Units 3)Separation Processes | Spring98-99 | 13 | 10 | **1.30** | 1.77 | 86 |
| MSE 192/202 (G Units 3)Solid StateThermodynamics | Autumn99-00 |  46 | 39 | **1.72** | 1.87 | 48 |
| ChE 444A (G Units 3)Quantum Simulations Molecules & Materials | Winter99-00 | 18 | 16 | **1.25** | 1.83 | 90 |
| ChE 130 (UG Units 3)Separation Processes | Spring99-00 | 18 | 16 | **1.25** | 1.78 | 87 |
| MSE 202 (G Units 3)Solid StateThermodynamics | Autumn00-01 |  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 | Spring00-01 | 20 | 13 | **1.23** | 1.73 | 90 |
| MSE 202 (G Units 3)Solid StateThermodynamics  | 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 | Spring01-02 | 32 | 30 | **1.33** | 1.77 | 78 |
| MSE 202 (G Units 3)Solid StateThermodynamics | Autumn02-03 | 24 | 21 | **2.42** | 1.77 | 19 |
| ChE 444A (G Units 3)Quantum Simulations Molecules & Materials | Winter02-03 | 13 | 12 | **1.25** | 1.65 | 84 |
| ChE 130 (UG Units 3)Separation Processes | Spring02-03 | 24 | 27 | **1.31** | 1.75 | 76 |
| ChE 444A (G Units 3)Quantum Simulations Molecules & Materials | Winter04-05 | 25 | 20 | **1.24** | 1.70 | 89 |
| ChE 130 (UG Units 3)Separation Processes | Spring04-05 | 27 | 25 | **1.48** | 1.72 | 64 |
| ChE 430 (G Units 3)Statistical Mechanics | Autumn05-06 | 50 | 50 | **2.3** | N/A | N/A |
| ChE 444A (G Units 3)Quantum Simulations Molecules & Materials | Winter05-06 | 40 | 25 | **1.2** | N/A | N/A |
| ChE 130 (UG Units 3)Separation Processes | Spring05-06 | 14 | 13 | **1.2** | N/A | N/A |
| ChE 430 (G Units 3)Statistical Mechanics | Autumn06-07 | 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 | Fall04-05 | 45 | 30 | **1.3** | NA | NA |

### 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 | Fall08-09 | 17 | 14 | **5.9** | 5.6 | 99 |
| CHEN 4330 (UG)Chemical Engineering Kinetics | Spring 08-09 | 49 | 44 | **5.3** | 4.7 | 68 |
| CHEN 4838Energy Fundamentals | Fall09-10 | 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 | Fall10-11 | 33 | 26 | **5.5** | 5.2 | NA |
| CHEN 4838 (UG)Energy Fundamentals | Fall10-11 | 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 | Fall11-12 | 38 | 28 | **5.2** | 5.1 | NA |
| **Course** | **Quarter Taught** | **Enrolled** | **Responses** | **Instructor Rating\*** | **Course Rating** | **Percentile** |
| CHEN 4330 (UG)Chemical Engineering Kinetics | Spring 11-12 | 41 | 18 | **5.7** | 5.3 | NA |
| CHEN 1211 (UG)Gen. Chemistry for Engineers | Fall12-13 | 441 | 182 | **3.8** | 3.9 | NA |
| CHEN 4838 (UG)Energy Fundamentals | Spring12-13 | 39 | 33 | **5.9** | 5.6 | NA |
| CHEN 1211 (UG)Gen. Chemistry for Engineers | Fall13-14 | 308 | 163 | **3.8** | 3.9 | NA |
| CHEN 4521 (UG)Physical Chemistry for Engineers | Spring13-14 | 188 | 140 | **3.1** | 2.8 | NA |
| CHEN 4521 (UG)Physical Chemistry for Engineers | Spring14-15 | 106 | 80 | **4.9** | 4.2 | NA |
| CHEN 4521 (UG)Physical Chemistry for Engineers | Spring14-15 | 98 | 82 | **3.9** | 3.5 | NA |
| CHEN 5838 (G)Quantum Simulations | Fall15-16 | 30 | 25 | **5.4** | 4.7 | NA |
| CHEN 4521 (UG)Physical Chemistry for Engineers | Spring15-16 | 91 | 78 | **4.6** | 4.2 | NA |
| CHEN 4521 (UG)Physical Chemistry for Engineers | Spring15-16 | 96 | 78 | **4.5** | 4.0 | NA |