Charles Bruce Musgrave
Associate Professor of Chemical and Biochemical Engineering
University of Colorado at Boulder
Boulder, CO

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

2012 –	Professor 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
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

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 NH_3 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 NH_3 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 NH_3," *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 ^{12}O and ^{11}B 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).

22. Kang, J. and C. Musgrave, "The Mechanism of HF/H_2O Chemical Etching of SiO_2," *Journal of Chemical Physics* 116, 275-280 (2002).

23. Kang, J. and C. Musgrave, "The Mechanism of Atomic Layer Deposition of SiO_2 on the Silicon (100)-2x1 Surface Using $SiCl_4$ and H_2O 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 O_2 and SiO_2 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).

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).

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).

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).

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).

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).

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).

34. Song, S., D. Golden, R. Hansen, C. Bowman, J. Senosiain, C. Musgrave, and G. Friedrichs, "A Shock Tube Study of the Reaction $NH_2 + CH_4 \rightarrow NH_3 + CH_3$ and Comparison with Transition State Theory," *International Journal of Chemical Kinetics* 35, 304-309 (2003).

35. Akis, R., D. Ferry, C. Musgrave, "Kinetic Lattice Monte Carlo Simulations of Processes on the Silicon (100) Surface," *Physica E-Low Dimensional Systems and Nanostructures* 19, 183-187 (2003).

36. Senosiain, J., C. Musgrave and D. Golden, "Temperature and Pressure Dependence of the Reaction of OH and CO: Master Equation Modeling on a High Level Potential Energy Surface," *International Journal of Chemical Kinetics* 35, 464-474 (2003).

37. Widjaja, Y., J. Han and C. Musgrave, "Quantum Chemical Study of Zirconium Oxide Deposition on the Si (100)-2x1 Surface," *Journal of Physical Chemistry B* 107, 9319-9324 (2003).

38. Mui, C., M. Filler, S. Bent, and C. Musgrave, "Reactions of Nitriles at Semiconductor Surfaces," *Journal of Physical Chemistry B* 107, 12256-12267 (2003).

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).

40. Han, J., G. Gao, Y. Widjaja, E. Garfunkel, and C. Musgrave, "A Quantum Chemical Study of ZrO_2 Atomic Layer Deposition Growth Reactions on the SiO_2 Surface," *Surface Science* 550, 199-212 (2004).

41. Xu, Y. and C. Musgrave, "A DFT Study of the Al_2O_3 Atomic Layer Deposition on SAMs: Effect of SAM Termination," *Chemistry of Materials*, 16, 646-653 (2004).

42. Pomerantz, A., J. Han, and C. Musgrave, "Calculating Cumulene/Poly-yne Isomerization Energies," *Journal of Physical Chemistry A*, 108, 4030-4035 (2004).

43. Heyman, A. and C. Musgrave, "A Quantum Chemical Study of Atomic Layer Deposition of Al_2O_3 Using $AlCl_3$ and H_2O as Precursors," *Journal of Physical Chemistry B*, 108, 5718-5725 (2004).

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).

45. Mui, C., S. Bent and C. Musgrave, "A Density Functional Theory Study on the Effect of Ge Alloying on Hydrogen Desorption from SiGe Alloy Surfaces," *Journal of Physical Chemistry B*, 108, 6336-6350 (2004).

46. Mui, C. and C. Musgrave, "Atomic Layer Deposition of HfO_2 Using Alkoxides as Precursors," *Journal of Physical Chemistry B*, 108, 15150-15164 (2004).

47. Mui, C., S. Bent and C. Musgrave, "A Quantum Chemistry Based Statistical Mechanical Model of Hydrogen Desorption from Si(100)-2x1, Ge(100)-2x1, and SiGe Alloy Surfaces," *Journal of Physical Chemistry B*, 108, 18243-18253, (2004).

48. Mui, C. and C. Musgrave, "Initial Oxidation and Hydroxylation of the Ge(100)-2x1 Surface by Water and Hydrogen Peroxide," *Langmuir*, 20, 7604-7609 (2004).

49. Yoon, T., C. Musgrave, S. Johnson and G. Brown, Jr., "Adsorption of Organic Matter at Mineral/Water Interfaces: I. ATR-FTIR Spectroscopic and Quantum Chemical Study of Oxalate Adsorbed at the Boehmite (γ-AlOOH)/Water and Corundum (α-Al_2O_3)/Water Interfaces," *Geochimica et Cosmochimica Acta*, 68, 4505-4518 (2004).

50. Centoni, S., B. Sadigh, G. Gilmer, T. de la Rubia and C. Musgrave, "First-Principles Calculation of Free Si(100) Surface Impurity Enrichment," *Applied Physics Letters*, 87, 232101-1-3 (2005).

51. Huang, K., J. Han, A. Cole, C. Musgrave and R. Waymouth, "Homolysis of Weak Ti-O Bonds: Experimental and Theoretical Studies of Titanium Oxygen Bonds Derived from Stable Nitroxyl Radicals," *Journal of the American Chemical Society*, 127, 3807-3816 (2005).

52. Centoni, S., B. Sadigh, G. Gilmer, T. Lenosky, T. de la Rubia and C. Musgrave, "First-Principles Calculation of Intrinsic Defect Formation Volumes in Silicon," *Physical Review B*, 72, 195206-1-9 (2005).

53. Xu, Y. and C. Musgrave, "Atomic Layer Deposition of Hafnium Nitrides Using Ammonia and Alkylamide Precursors," *Chemical Physics Letters*, 407, 272-275 (2005).

54. Mui, C. and C. Musgrave, "Thermal Nitridization of the Ge(100) 2x1 Surface By Ammonia," *Langmuir*, 21, 5230-5232 (2005).

55. Xu, Y. and C. Musgrave, "Atomic Layer Deposition of HfO_2 on Nitridized Si Surfaces," *Applied Physics Letters*, 86, 192110-192113 (2005).

56. Xu, Y. and C. Musgrave, "A Chemical Mechanism for Nitrogen Incorporation Into HfO_2 ALD Films Using Ammonia and Alkylamides as Precursors," *Surface Science, 591, L280-L285* (2005).

57. Kelly, M., J. Han, C. Musgrave and G. Parsons, "In-Situ Infrared Spectroscopy and Density Functional Theory Modeling of Hafnium Alkylamine Adsorption on Si-OH and Si-H Surfaces," *Chemistry of Materials*, 17, 5305-5314 (2005).

58. Solares, S., S. Dasgupta, Y. Kim, C. Musgrave, P. Schultz, and W. Goddard, "Density Functional Theory Study of the Geometry, Energetics and Reconstruction Process of Si(111) Surfaces," *Langmuir*, 21, 12404-12414 (2005).

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).

60. Mukhopadhyay, A. and C. Musgrave, "Non-Growth Ligand Exchange Reactions in Atomic Layer Deposition of HfO_2," *Chemical Physics Letters*, 421, 215-220 (2006).

61. Mukhopadhyay, A., J. Sanz and C. Musgrave, "First-Principles Calculations of Structural and Electronic Properties of Monoclinic Hafnia Surfaces," *Physical Review B*, 73, 115330-115337 (2006).

62. Huang, K., J. Han, C. Musgrave, and R. Waymouth, "Density Functional Theory Calculations on Ti-TEMPO Complexes: Influence of Ancillary Ligation on the Strength of the Ti-O bond," *Organometallics*, 25, 3317-3323 (2006).

63. Mukhopadhyay, A., J. Sanz and C. Musgrave, "First-Principles Investigation of Hydroxylated Monoclinic HfO_2 Surfaces," *Chemistry of Materials*, 18, 3397-3403 (2006).

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).

65. Huang, K., J. Han, C. Musgrave, and E. Fujita, "Carbon Dioxide Reduction by Pincer Rhodium η^2-Dihydrogen Complexes: Hydrogen Binding Modes and Mechanistic Studies by Density Functional Theory Calculations," *Organometallics*, 26, 508-513, (2007).

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).

67. Zhang, G. and C. Musgrave, "Comparison of DFT Methods for Molecular Orbital Eigenvalue Calculations," *Journal of Physical Chemistry A*, 111, 1554-1561 (2007).

68. Ardalan, P., N. Davani and C. Musgrave, "The Attachment of Alanine and Arginine to the Ge(100)-2x1 Surface," *Journal of Physical Chemistry C*, 111, 3692-3699 (2007).

69. Mukhopadhyay, A. and C. Musgrave, "The Role of Ammonia in the Atomic Layer Deposition of Tungsten Nitride," *Applied Physics Letters*, 90, 173120-173122 (2007).

70. Mukhopadhyay, A., J. Sanz and C. Musgrave, "First-Principles Investigation of the Structure, Energetics and Electronic Properties of Ru/HfO_2 Interfaces," *Journal of Physical Chemistry C*, 111, 9203-9210 (2007).

71. Paul, A., and C. Musgrave, "Catalyzed Dehyrdogenation of Ammonia-Borane by Iridium Dihydrogen Pincer Complex Differs from Ethane Dehydrogenation," *Angewandte Chemie*, 46, 8153-8156 (2007).

72. Ha, Y, T. Yoon, Y. Wang, C. Musgrave and G. Brown, "Adsorption of Organic Matter at Mineral/Water Interfaces: 7. ATR-FTIR and Quantum Chemical Study of Lactate Interactions with Hematite Nanoparticles," *Langmuir*, 24, 6683-6692 (2008).

73. Flory, C., C. Musgrave and Z. Zhang, "Quantum Dot Properties in the Multiband Envelope-Function Approximation Using Boundary Conditions Based Upon First-Principles Quantum Calculations," *Physical Review B*, 77, 205312-205324 (2008) and *Virtual Journal of Nanoscale Science and Technology*, 17, (2008).

74. Mukhopadhyay, A., C. Musgrave and J. Sanz, "Atomic Layer Deposition of Hafnium Oxide from Hafnium Chloride and Water," *Journal of the American Chemical Society*, 130 11996-12006 (2008).

75. Zimmerman, P., A. Paul, Z. Zhang and C. Musgrave, "Oligomerization and Autocatalysis of NH_2BH_2 with Ammonia-Borane," *Inorganic Chemistry*, 48, 1069-1081 (2009).

76. Ardalan, P., C. Musgrave and S. Bent, "Formation of Alkanethiolate Self-Assembled Monolayers at Halide-Terminated Ge Surfaces," *Langmuir*, 25, 2013-2025 (2009).

77. Zimmerman, P., A. Paul, Z. Zhang, and C. Musgrave, "The Role of Free N-Heterocyclic Carbene in the Catalytic Dehydrogenation of Ammonia-Borane in the Ni NHC System," *Angewandte Chemie International Edition*, 48, 2201-2205 (2009).

78. Zimmerman, P., A. Paul, and C. Musgrave, "Catalytic Dehydrogenation of Ammonia Borane at Ni Monocarbene and Dicarbene Catalysts," *Inorganic Chemistry*, 48, 5418-5433 (2009).

79. Zimmerman, P., J. Toulouse, Z. Zhang, C. Musgrave and C. Umrigar, "Excited States of Methylene from Quantum Monte Carlo," *Journal of Chemical Physics*, 131, 124103 (2009).

80. Mukhopadhyay, A., J. Fernandez. Sanz and C. Musgrave, "Effect of Interface Structure on the Ru on HfO_2 Work Function," *Journal of Materials Science*, (2010).

81. Ardalan, P., Y. Sun, P. Pianetta, C. Musgrave, and S. Bent, "Reaction Mechanism, Bonding and Thermal Stability of 1-Alkanethiols Self-Assembled on Halogenated Ge Surfaces," *Langmuir*, 26 (11) 8419-8429 (2010).

82. Zimmerman, P., Z. Zhang, and C. Musgrave, "Generation of Multiple Triplet Excitons in Pentacene by Singlet Fission Through Doubly-Excited Dark States," *Nature Chemistry, 2*, 648-652 (2010). *Nature Chemistry Highlighted Article.*

83. Zimmerman, P., Z. Zhang, and C. Musgrave, "Concerted Two Hydrogen Transfer As An Effective Mechanism for Selective CO_2 Reduction," *Inorganic Chemistry*, 49, 8724-8728 (2010).

84. Pelz, K., C. Musgrave, J. Falconer and J. Medlin, "Effects of Water and Formic Acid Adsorption on the Electronic Structure of Anatase TiO_2 (101)," *Journal of Chemical Physics C*, 115 (6), 2738-2749 (2011). DOI: 10.1021/jp109014a

85. Zimmerman, P., Z. Zhang and C. Musgrave," Dynamic Mechanisms For Ammonia Borane Thermolysis In Solvent: Deviation From Gas Phase Minimum Energy Pathway," *Journal of Physical Chemistry Letters*, 2, 276-281 (2011). DOI: 10.1021/jz101629d

86. Ardalan, P., G. Dupont and C. Musgrave, "Reactions of Amino Acids on the Si(100)-2x1 Surface," *Journal of Physical Chemistry C*, 115, 7477-7486 (2011). DOI: 10.1021/jp1114702

87. Somani, S., A. Mukhopadhyay and C. Musgrave, "Atomic Layer Deposition of Tantalum Nitride Using A Novel Precursor," *Journal of Physical Chemistry C*, 115, 11507-11513 (2011). DOI: 10.1021/jp1059374

88. Muhich, C., Y. Zhou, A. Holder, A. Weimer and C. Musgrave, "The Effect of Surface Deposited Pt on the Photactivity of TiO_2," *Journal of Physical Chemistry C, 116, 10138-10149 (2012).* DOI: 10.1021/jp301862m

89. Zhou, Y., C. Muhich, B. Neltner, A. Weimer and C. Musgrave, "Growth of Pt Particles on the Anatase TiO_2 Surface," *Journal of Physical Chemistry C*, (2012). DOI: 10.1021/jp302273m

INVITED 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 ZrO_2 Atomic Layer Deposition on the SiO_2 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*, Submitted, November 2010.

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 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
Department Fundraising and Alumni Relations Committee
Biotechnology Building Design Committee - Computer Server Room
East Campus Master Plan Vision Subcommittee 2010
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 2011-

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.

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

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.

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.

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 Nanostructrues, 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-P_J) with H_2O_2: 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., "HfO_2 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 HfO_2,” *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 HfO_2,” *American Chemical Society National Meeting*, Boston, MA, August 2007.

45. Mukhopadhyay, A., Sanz, J. and Musgrave, C., “Molecular Dynamics Simulations of HfO_2 Atomic Layer Deposition,” *American Vacuum Society Annual Meeting*, Seattle, WA 2007.

46. Mukhopadhyay, A., Zhang, Z. and Musgrave, C., “Simulations of HfO_2 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 Al_2O_3 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., 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.

56. Musgrave, C., "Guiding Principles For The Catalytic Reduction Of CO_2 From Theory," American Chemical Society Fall National Meeting, Denver, CO, August 2011.

57. Musgrave, C., "Singlet Fission in Organic Photovoltaics," American Physical Society March National Meeting, Boston, MA, February 2012.

58. Musgrave, C., "Chemical Mechanisms of Atomic Layer Deposition from First Principles Calculations," American Chemical Society Spring National Meeting, San Diego, CA, March 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,” I-CAMP Summer School, Boulder, CO, July 2012.

61. Musgrave, C., “Excited States: How to Properly Describe Excited States,” I-CAMP Summer School, Boulder, CO, July 2012.

62. Musgrave, C., “Excited State Processes: Conical Intersections, Conversions, Couplings, Crossings, etc.,” I-CAMP Summer School, Boulder, CO, July 2012.

63. Musgrave, C., “Exciton Multiplication: The Mechanism of Singlet Fission in OPV,” I-CAMP Summer School, Boulder, CO, July 2012.

DEPARTMENT SEMINARS

1. Musgrave, C., “Ab Initio Simulations for Film Growth and Polymer Force Fields,” *Department of Chemical Engineering Colloquium*, Stanford, CA, April 1994.

2. Musgrave, C., “Development of Molecular Mechanics Potentials and Simulations of Diamond Chemical Vapor Deposition and Nanotechnology,” *Department of Materials Science Colloquium*, North Carolina State University, Raleigh, NC, October 1994.

3. Musgrave, C., “Ab Initio Studies of the Manipulation of Reactivity of Surfaces Using STM for Growing Nanostructures and Diamond Chemical Vapor Deposition,” Oak Ridge National Laboratory, Oak Ridge, TN, October 1995.

4. Musgrave, C., “Quantum Chemistry of In Situ Doping of Si CVD,” *Department of Materials Science and Engineering Colloquium*, Stanford University, Stanford, CA, November 1996.

5. Musgrave, C., “The Adsorption and Decomposition of Phosphine on Si(100),” NASA Moffett Field, Mountain View, CA, March 1997.

6. Musgrave, C., “Ab Initio Simulations of Semiconductor Processing Chemistry,” *Department of Chemical Engineering Colloquium*, Stanford, CA, March 1999.

7. Musgrave, C., “Cluster Simulations of Silicon Surface Chemistry: Is Charge Transfer a Non-local Effect?,” Lawrence Livermore National Laboratory, Livermore, CA, May 1999.

8. Musgrave, C., “Prediction of Chemical Mechanisms for Semiconductor Processing,” *Department of Chemical Engineering Colloquium*, University of Illinois, Urbana, IL, February 2000.

9. Widjaja, Y., and C. Musgrave, “Silicon Nitride Deposition Using Ammonia,” *Department of Chemical Engineering,* Stanford University, Stanford, CA, October 2000.

10. Senosiain, J., C. Musgrave, D. M. Golden, “Reaction of OH and O (3-P_J) with H_2O_2: 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., "Quantum Simulations for Energy Applications: Carrier Multiplication in Organic Photovoltaics and Catalytic Reduction of CO_2," Department Seminar, Department

of Chemical Engineering, Brigham Young University, September 2011.

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 ZrO_2 and HfO_2 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 ZrO_2 and HfO_2 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 HfO_2 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.

CONFERENCE PRESENTATIONS

1. Musgrave, C., "Development of Molecular Mechanics Potentials from First Principles: The Si(111)-7x7 Reconstruction," *West Coast Theoretical Chemistry Conference*, Salt Lake City, UT, May 1990.

2. Musgrave, C., "Molecular Mechanics Simulations of the Dimer Adatom Stacking Fault (2n+1) x (2n+1) Reconstructions of (111) Silicon," *American Conference of Theoretical Chemistry*, San Diego, CA, June 1990.

3. Musgrave, C., "A Hydrogen Abstraction Tool for Nanotechnology," *Foresight Conference on Nanotechnology*, Palo Alto, CA, November 1991.

4. Musgrave, C., "Ab Initio Simulations of the Chemical Vapor Deposition of Diamond," *West Coast Theoretical Chemistry Conference*, Mountain View, CA, May 1992.

5. Musgrave, C., and M. Mysinger, "First Principles Study of Phosphine Adsorption and Decomposition on Si(100)-2x1," *American Institute of Chemical Engineers Annual Meeting*, Miami, FL, November 1998.

6. Musgrave, C., "Adhesion, Dynamics and Degradation of PFPE Hard Disk Lubricants," Center on Polymer Interfaces and Macromolecular Assemblies (CPIMA) Forum, Department of Chemical Engineering, Stanford University, Stanford, CA, August 1999.

7. Ricca, A., and C. Musgrave, "Modeling Silicon Surface Chemistry with Clusters: Chlorine on the Si(100)-2x1 and (111) Surfaces," *American Institute of Chemical Engineers Annual Meeting*, Miami, FL, November 1998.

8. Mysinger, M., A. Ricca, and C. Musgrave, "A Quantum Chemical Study of the Chemistry of Silicon Surfaces: Cl, Phosphine and Ammonia on Silicon," *American Institute of Chemical Engineers Annual Meeting*, Miami, FL, November 1998.

9. Senosiain, J., D. Golden, and C. Musgrave, "Use of Ab Initio Quantum Mechanics To Estimate Rate Constants," US-German Environmental Chamber Workshop, University of California, Riverside, CA, October 1999.

10. Mui, C., S. Bent, and C. Musgrave, "Theoretical Approach for Predicting $Si_{x-1}Ge_x$ Surface Chemistry," *American Institute of Chemical Engineers Annual Meeting*, Dallas, TX, November 1999.

11. Kang, J., and C. Musgrave, "The KMLYP Density Functional Approximation: A New Method for Accurate Prediction of Activation Barriers and Enthalpies of Reaction," *AVS 48th International Symposium*, Boston, MA, October 2000.

12. J. Kang, and C. Musgrave, "A New Method for the Accurate Prediction of Activation Barriers and Enthalpies of Reaction, American Institute of Chemical Engineering," Los Angeles, CA, November 2000.

13. Senosiain, J., D. Golden, J. Kang, and C. Musgrave, "Use of Ab Initio Quantum Methods and Transition State Theory to Estimate Rate Constants for Computational Prototyping," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.

14. Kang, J. and C. Musgrave, "A Theoretical Study of the Chemical Vapor Deposition of (100) Diamond: An Explanation for the Slow Growth of the (100) Surface," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.

15. Mui, C., S. Bent, and C. Musgrave, "Theoretical Predictions for SiGe Heteroepitaxy," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.

16. Widjaja, Y. and C. Musgrave, "Quantum Chemical Study of Silicon Nitride Deposition Using Ammonia," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.

17. Kang, J. and C. Musgrave, "The KMLYP Hybrid DFT Method: A Chemically Accurate Method for Understanding Reactivity," *American Institute of Chemical Engineers Annual Meeting*, Los Angeles, CA, November 2000.

18. Widjaja, Y. and C. Musgrave, "An Ab Initio Study of the Initial Oxidation of the Silicon (100)-2x1 Surface," *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.

19. Widjaja, Y. and C. Musgrave, "An Ab Initio Study of the Initial Oxidation of Si(100)-(2x1)," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

20. Musgrave, C. and J. Kang, "A Theoretical Study Of The Chemical Vapor Deposition Of (100) Silicon From Silane," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

21. Musgrave, C. and Y. Widjaja, "Quantum Chemical Study of Zirconium Oxide Atomic Layer Deposition: Gas Phase and Surface Reactions," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

22. Musgrave, C. and J. Kang, "Nanometer Scale Manipulation of Surface Reaction Kinetics by STM Electric Fields: A Density Functional Theory Study," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

23. C. Musgrave, "Teaching Quantum Chemical Simulations in Chemical Engineering," *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

24. Kang, J. and C. Musgrave, "Prediction of Accurate Reaction Barriers and Enthalpies of Reaction by a New Hybrid DFT Method," Poster Presentation, *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

25. Senosiain, J., D. Golden, and C. Musgrave, "Tunneling Effects in Bimolecular Chemical Reactions," Poster Presentation, *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

26. Prinz, P. and C. Musgrave, "Low Temperature Solid Oxide Fuel Cells," *2002 Office of Naval Research: Materials Review*, Woods Hole, MA, May 2002.

27. Widjaja, Y. and C. Musgrave, "Quantum Simulations of Growth of High-K Gate Stacks," *American Institute of Chemical Engineers Annual Meeting*, Indianapolis, IN, November 2002.

28. Mui, C., C. Musgrave, and S. Bent, "Hydrogen Desorption from (100) 2x1 Silicon, Germanium and SiGe Alloy Surfaces," *American Institute of Chemical Engineers Annual Meeting*, Indianapolis, IN, November 2002.

29. Mui, C. and C. Musgrave, and S. Bent, "Organic Functionalization of Silicon and Germanium Surfaces," *American Institute of Chemical Engineers Annual Meeting*, Indianapolis, IN, November 2002.

30. Senosiain, J., J. Kang, D. Golden, and C. Musgrave, "A Critical Analysis of Quantum Chemical Methods for the Prediction of Kinetics and Thermochemical Properties," *American Institute of Chemical Engineers Annual Meeting*, Indianapolis, IN, November 2002.

31. Musgrave, C. and J. Han, "ALD of High-K Gate Materials on Si, Ge and SiGe Alloy Materials for 3-D Microelectronics," MARCO Materials, Structures and Devices Center Teleconference, Massachusetts Institute of Technology, Cambridge, MA, April 2003.

32. Musgrave, C., Y. Widjaja, and J. Han, "Atomistic Simulations of Surface Chemical Reactions for Growing High-K Gate Stacks," Materials Research Society Spring Meeting, San Francisco, CA, April 2003.

33. Musgrave, C., "Quantum Chemical Simulations for Nanoelectronics: Materials by Design," *NSF Nanoscience Young Scientist Exchange Program*, Tokyo University, Tokyo, Japan, November 2003.

34. Xu, Y., and C. Musgrave, "Quantum Simulation of Thin Film Growth for 3D Microelectronic Devices," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

35. Musgrave, C., "ALD of High-K Dielectrics with Alkylamide Precursors," *MARCO Materials Structures and Devices Center Review*, Massachusetts Institute of Technology, Cambridge, MA, April 2004.

36. Han, J., M. Kelly, C. Musgrave and G. Parsons, "DFT Study of the Initial ALD Reactions of $Hf(N(CH_3)_2)_4$ on the Si-H Surface: Chemical Mechanism and Vibrational Spectra," *The Fourth American Vacuum Society Topical Conference on Atomic Layer Deposition*, Helsinki, Finland, August 2004.

37. Han, J. and C. Musgrave, "Quantum Chemical Simulations of ALD of HfO_2 Using Hafnium Alkylamide Precursors," *The Fourth American Vacuum Society Topical Conference on Atomic Layer Deposition*, Helsinki, Finland, August 2004.

38. Han, J., S. Wang, R. Gordon and C. Musgrave, "Kinetics of HfO_2 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 $Hf(N(CH_3)_2)_4$ on the SiO_2 and Si-H Surfaces: Mechanism, Kinetics, Vibrational Spectra and Interface Structure," *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.

41. Xu, Y. and C. Musgrave, "ALD of High-K Dielectrics on Nitrided Si and Ge Surfaces," *American Institute of Chemical Engineers Annual Meeting*, Austin, TX, November 2004.

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.

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46. Dupont, G. and C. Musgrave, "Electronic Coupling of Organics to Semiconductors Through Quantum Resonance," *American Physical Society March Meeting*, Los Angeles, CA, March 2005.

47. Han, J. and C. Musgrave, "Density Functional Theory Simulations of Atomic Layer Deposition of HfO_2," *American Physical Society March Meeting*, Los Angeles, CA, March 2005.

48. Dupont, G. and C. Musgrave, "DFT Study of Amino Acids on Si Surface for Hybrid Organic-Semiconductor and Protein-Semiconductor Structures," *American Physical Society March Meeting*, Los Angeles, CA, March 2005.

49. Mui, C. Y. Xu, and C. Musgrave, "DFT Simulations of the Growth of Thin Films on Si and Ge," *American Physical Society March Meeting*, Los Angeles, CA, March 2005.

50. Dupont, G. and C. Musgrave, "Organic Functionalization of Semiconductors Using Amino Acids: Quantum Resonance Coupling and Electron Transport Effects," *American Vacuum Society Annual Meeting*, Boston, MA, November 2005.

51. Mukhopadhyay, A., J. Han and C. Musgrave, "Chemical Mechanisms of Contamination in Atomic Layer Deposition of HfO_2," *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 HfO_2," *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 HfO_2," *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 RuO_2 on HfO_2 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 HfO_2," *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," *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 Al_2O_3 Coherent Superconducting Phase Qubit Dielectrics, " *Coherent Superconducting Qubit Meeting*, San Diego, CA, January, 2011.

67. Musgrave, C., C. Lim, A. Holder, C. Bowman, "Design and Implementation of Novel Photoinitiators," Industry University Collaborative Research Center, St. Paul, MN, April 2012.

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 NH_3 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 NH_3 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 NH_3 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 SiO_2 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 $(Ba,Sr)TiO_3$ Film precursors,” *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.

22. Widjaja, Y. and C. Musgrave, Quantum Chemical Study of Zirconium Oxide Atomic Layer Deposition,” *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.

23. Wang, G., C. Mui, C. Musgrave and S. Bent, “Probing the Selectivity of Multifunctional Compounds on Semiconductor Surfaces: Pyrrole and its Derivatives on Si and Ge (100)-2x1,” *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.

24. Mui, C., G. Wang, C. Musgrave and S. Bent, “Are Silicon and Germanium Surfaces Chemically Similar? Reactions of Amines,” *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.

25. Kang, J. and C. Musgrave, “A Theoretical Study of The Chemical Vapor Deposition of (100) Silicon From Silane,” *American Vacuum Society Annual Meeting*, San Francisco, CA, October 2001.

26. Wang, G., C. Mui, C. Musgrave and S. Bent, "Competition and Selectivity of Organic Reactions on Semiconductor Surfaces," *16th Annual William S. Johnson Symposium in Organic Chemistry*, Stanford University, CA, October 2001.

27. Wang, G., C. Mui, C. Musgrave and S. Bent, “Probing the Reactivity of Amines on Si(100)-2x1 and Ge(100)-2x1 Surfaces,” *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

28. Musgrave, C. and Y. Widjaja, “A DFT Study of the Initial Growth Mechanism of Silicon Nitride on Si(100)-(2x1) Using Ammonia and Atomic Nitrogen,” *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

29. Widjaja, Y. and C. Musgrave, Quantum Chemical Study of Zirconium Oxide Atomic Layer Deposition on the Si(100)-(2x1) Surface,” *American Institute of Chemical Engineers Annual Meeting*, Reno, NV, November 2001.

30. Wang, G., C. Mui, C. Musgrave and S. Bent, "Competition and Selectivity of Organic Reactions on Semiconductor Surfaces," *5th Annual Flory Conference in Macromolecular and Physical Chemistry*, Stanford, CA, February 2002.

31. Senosiain, J. and C. Musgrave, "Atomic Layer Deposition of High-K Gate Dielectrics on Germanium," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS,* Stanford University, June 2002.

32. Chen, R., Y. Widjaja, G. Gao and C. Musgrave, "Atomic Layer Deposition of High-K Gate Dielectrics," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS,* Stanford University, June 2002.

33. Filler, M., C. Mui, G. Wang, C. Musgrave and S. Bent, "Gaining Molecular and Atomic Level Control of Semiconductor Interfaces through Organic Functionalization," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS,* Stanford University, June 2002.

34. Mui, C., S. Bent and C. Musgrave," Organic Chemistry at Semiconductor Surfaces Studied by FTIR and DFT," IBM Storage Division, San Jose, CA July 2002.

35. Mui, C., S. Bent and C. Musgrave," Organic Chemistry at Semiconductor Surfaces Studied by FTIR and DFT," SRI International, Menlo Park CA, December 2002.

36. Senosiain, J., D. Golden and C. Musgrave, "Modeling the kinetics of OH+CO: A Stochastic Approach," Sandia National Laboratory, Livermore, CA, August 2002.

37. Chen, R., C. Mui, S. Bent and C. Musgrave, "Area Selective Atomic Layer Deposition (ALD) of High-K Dielectrics," *Annual Retreat NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing*, Stanford CA, August 2002.

38. Kawakami, B., C. Musgrave, M. Reinhard, and P. Roberts, "Enzyme Reaction Modeling of Hazardous Pollutant Transformation: Structural Basis of Biodegradability," *Biomedical Computation at Stanford Conference*, Stanford University, Stanford, CA, October 2002.

39. Filler, M., C. Mui, C. Musgrave and S. Bent, "Modifying the Semiconductor Interface with Organonitriles," *49th Annual Meeting of the American Vacuum Society*, Denver, CO, November 2002.

40. Chen, R., J. Han, C. Mui, S. Bent and C. Musgrave, "Area Selective ALD of High-K Dielectrics," *Annual Retreat NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing*, Tucson AZ, February 2003.

41. Bent, S., Chen, R., C. Mui and C. Musgrave, "A Theoretical Investigation of Area Selective Atomic Layer Deposition of High-K Dielectrics," *Annual Retreat NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing*, Tucson AZ, February 2003.

42. Chen, R., J. Han, C. Mui, S. Bent, and C. Musgrave, "An Experimental and Theoretical Investigation of Selective Area ALD of High-K Dielectrics," Flory Conference, Stanford, CA, February 2003.

43. Han, J., Y. Widjaja, R. Chen, S. Bent, R. Gordon, G. Gao and C. Musgrave, "A DFT Study of Atomic-Layer Deposition for ZrO_2 and HfO_2," Flory Conference, Stanford, CA, February 2003.

44. Huang, K., J. Han, Y. Widjaja, C. Musgrave, and R. Waymouth, "The Role of the Oxidation State of Titanium and Solvent Effects in Ethylene/Styrene Copolymerization: A DFT Theoretical Study," Flory Conference on Novel Electronic Materials, Stanford, CA, February 2003.

45. R. Pornprasertsuk, C. Musgrave and F. Prinz, "DFT Simulations of Oxygen Transport Through ZrO_2 for Low-T Solid Oxide Fuel Cells," Flory Conference, Stanford, CA, February 2003.

46. Xu, Y. and C. Musgrave, "Quantum Simulation of Thin Film Growth for 3-D Microelectronics," Flory Conference on Novel Electronic Materials, Stanford, CA, February 2003.

47. Mui, C., S. Bent and C. Musgrave, "A Theoretical Study on Hydrogen Desorption from SiGe Alloy Surfaces," Flory Conference, Stanford, CA, February 2003.

48. Mui, C., S. Bent and C. Musgrave. "Organic Chemistry at Semiconductor Surfaces Studied by FTIR and DFT," Lam Research Corporation, Fremont CA, May 2003.

49. Han, J., S. Wang, R. Gordon and C. Musgrave, "Kinetics and Thermodynamics of Atomic Layer Deposition of High-κ Dielectrics using Alternative Metallorganic Precursors," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS,* Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.

50. Xu, Y. and C. Musgrave, "Quantum simulation of Thin Film Growth for 3-D Microelectronic Device," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS,* Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.

51. Heyman, A. and C. Musgrave, "Density Functional Theory Calculations of Atomic Layer Deposition of Al_2O_3 from $AlCl_3$ and H_2O Precursors," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS,* Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.

52. Mui, C., J. Han and C. Musgrave, "Quantum Chemical Studies of Atomic Layer Deposition of Hafnium Oxide," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS,* Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.

53. Chen, R., H. Kim, C. Musgrave, P. McIntyre and S. Bent, "Surface Modification for Area-Selective Atomic Layer Deposition," *Nano and Bio-Nanoscience Research Meeting, Northern California Chapter of the AVS,* Lawrence Berkeley National Laboratory, Berkeley, CA, June 2003.

54. Mui, C., S. Bent and C. Musgrave. "Organic Chemistry at Semiconductor Surfaces Studied by FTIR and DFT," Hitachi Global Storage Technologies, San Jose CA, June 2003.

55. Mui, C. and C. Musgrave, "Quantum Chemical Studies of Atomic Layer Deposition of Hafnium Oxide," Novellus Systems Incorporated, San Jose CA, June 2003.

56. Mui, C. and C. Musgrave, "Quantum Chemical Studies of ALD of Hafnium Oxide Using Alkoxide Precursors," Applied Materials Corporation, San Jose CA, July 2003.

57. Mui, C. and C. Musgrave, "Atomic Layer Deposition of Hafnium Oxide Using Alkoxide Precursors," Intel Corporation, San Jose CA, July 2003.

58. Han, J., S. Wang, R. Gordon, and C. Musgrave, “Atomic Layer Deposition of High-k Dielectrics using Alternative Metallorganic Precursors,” *Initiative for Nanoscale Materials Processing Metal Gate-Metal Workfunction Meeting,* Stanford University, Stanford, CA, August 2003.

59. Xu, Y. and C. Musgrave, “ALD of Metals and Metal Oxides on Organics for Organic and Molecular 3D Electronics,” *Nano and Bio-Nanoscience Research Meeting, Initiative for Nanoscale Materials Processing Metal Gate-Metal Workfunction Meeting,* Stanford University, Stanford, CA, August 2003.

60. Heyman, A. and C. Musgrave, “DFT Study of ALD of Al_2O_3 from $AlCl_3$ and H_2O Precursors,” *Initiative for Nanoscale Materials Processing Metal Gate-Metal Workfunction Meeting,* Stanford University, Stanford, CA, August 2003.

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62. Heyman, A. and C. Musgrave, “Density Functional Theory Calculations of Atomic Layer Deposition of Al_2O_3 from $AlCl_3$ and H_2O Precursors,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

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65. Pornprasertsuk, R., J. Cheng, Y. Sata, F. Prinz and C. Musgrave, “Quantum Simulation Studies of Oxygen Ion Diffusion in Solid Oxide Fuel Cell Electrolytes,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

66. Walther, J. and C. Musgrave, “Quantum Chemical/Molecular Mechanical Study of the Reaction Mechanism of Peptide Bond Hydrolysis as Catalyzed by Chymotrypsin,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

67. Huang, K., J. Han, Y. Widjaja, C. Musgrave and R. Waymouth, “The Role of the Oxidation State of Titanium and Solvent Effects in Ethylene/Styrene Copolymerization: A DFT Theoretical Study,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

68. Xu, Y. and C. Musgrave, “Quantum Simulations of Thin Film Growth for 3-D Microelectronic Devices,” *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2003.

69. Han, J. and C. Musgrave, “Atomic Layer Deposition of High-□ Dielectrics using Alternative Metallorganic Precursors,” *Initiative for Nanoscale Materials Processing Annual Review*, Stanford University, Stanford, CA, November 2003.

70. Mui, C., Y. Xu and C. Musgrave, "Atomic Layer Deposition on Silicon, Germanium and Self-Assembled Monolayers," *Initiative for Nanoscale Materials Processing Annual Review*, Stanford University, Stanford, CA, November 2003.

71. Han, J., K. Huang, R. Waymouth and C. Musgrave, "Quantum Chemical Studies of HfO_2 Atomic Layer Deposition and Titanium-TEMPO Polymerization Catalysis," Exxon Mobil Corporation, Alexandria, VA, January 2004.

72. Han, J., K. Huang, R. Waymouth and C. Musgrave, "DFT Studies of the Metallorganic Chemistry of Titanium-TEMPO Polymerization Catalysis and HfO_2 Atomic Layer Deposition," Rohm and Haas Corporation, Spring House, PA, January 2004.

73. Han, J., K. Huang, R. Waymouth and C. Musgrave, "A DFT Investigation of HfO_2 Atomic Layer Deposition and Titanium-TEMPO Polymerization Catalysis," Exxon Mobil Corporation, Houston, TX, February 2004.

74. Han, J. and C. Musgrave, "ALD of High-k Dielectrics with Alkylamide Precursors," Initiative for Nanoscale Materials Processing *Nanoscale Materials Characterization Workshop*, Stanford University, Stanford, CA, February 2004.

75. Han, J., K. Huang, R. Waymouth and C. Musgrave, "DFT Simulations of ALD of HfO_2," Intel Corporation, Santa Clara, CA, February 2004.

76. Xu, Y. and C. Musgrave, "ALD on Self-Assembled Monolayers for 3-D Microelectronic Devices and Molecular Electronics," Initiative for Nanoscale Materials Processing *Nanoscale Materials Characterization Workshop*, Stanford University, Stanford, CA, February 2004.

77. Han, J., K. Huang, R. Waymouth and C. Musgrave, "DFT Simulations of ALD of HfO_2 and Titanium-TEMPO Polymerization Catalysis," Exxon Mobile Corporation, Fairfax, VA, March 2004.

78. Xu, Y. and C. Musgrave, "ALD on Self-Assembled Monolayers for Area Selective ALD," Initiative for Nanoscale Materials Annual Review, Stanford, CA, May 2004.

79. Han, J. and C. Musgrave, "ALD of High-k Dielectrics Using Metalorganic Precursors," Initiative for Nanoscale Materials Annual Review, Stanford, CA, May 2004.

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