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Personal Data

Date of Birth: October 19, 1952 Place of Birth: Greenville, NC, USA
Marital Status: Single

Education

Universities	Major	Degree
Arizona State University Tempe, AZ	Physics (Solid State Theory)	Ph.D. Aug., 1992 (GPA 3.76/4.00)
North Carolina State University Raleigh, NC	Physics (Nuclear)	M.S. Dec., 1983
University of North Carolina Chapel Hill, NC	Physical Education	M.A. Dec., 1977
University of North Carolina Chapel Hill, NC	Mathematics	B.S. Aug., 1972

Employment

8/05 - present	Lecturer, Dept. of Physics, ASU
6/99 - 8/05	Physics Instructor, ASU
7/98 - 2/99	Consulting Faculty, Materials Research Science and Engineering Center, ASU
5/98 - 7/98	Physics Instructor, ASU
7/97 - 11/97	Postdoctoral Research Faculty, ASU
1/96 - 7/97	Physics Instructor, ASU
9/92 - 9/94	Postdoctoral Research Faculty, ASU
8/85 - 8/92	Teaching or Research Assistant, ASU
8/84 - 6/85	Physics, Math, and Physical Education Teacher, Good Hope School, St. Croix, USVI
1/84 - 7/84	Physics Instructor North Carolina State University
6/82 - 12/83	Research Assistant, Triangle Universities Nuclear Laboratory, Durham NC
8/80 - 5/82	Teaching Assistant, NCSU
8/79 - 6/80	Physics and Math Teacher, Parker School, Kamuela HI
8/78 - 6/79	Math Teacher, Hawaii Preparatory Academy, Kamuela HI

Honors and Awards

5/06	Invited Talk on "First-Principles Quantum Molecular Dynamics" as a part of the Spring Seminar Series at Colby College in Waterville, Maine.
4/04	Invited Talk on "Fullerene Polymerization", as a part of the Spring 2004 Soft Matter Seminar Series, Department of Physics and Astronomy, Arizona State University, Tempe AZ.
11/03	Invited Talk on "The Odd-Numbered Fullerene Derivatives C_{119} and C_{139}", Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, H-1525 Budapest, Hungary
1/98	Invited Chapter on "First Principles Molecular Dynamical Studies of Polymerized C_{60}" as a part of "*Fullerene Polymers and Fullerene-Polymer Composites*" (Springer Verlag, Berlin) 2000, pp. 185 - 227.
1/95	Invited Talk on "First Principles Molecular Dynamics Simulations of Silicon Surfaces and Carbon Fullerenes" as a part of the Spring Colloquium Series, Florida Institute of Technology, Melbourne, FL.
5/94	Invited Talk on "Local-Orbital-Based Quantum Molecular Dynamics Simulations of C_{60} on Silicon Surfaces", at the Electrochemical Society Spring meeting, San Francisco, CA.
10/93	Invited Talk on "A First Principles Molecular Dynamical Study of Polymerized C_{60} and of C_{119}", at the Electrochemical Society Fall meeting, New Orleans, LA.
4/93	Invited Talk on the "Jahn-Teller Interactions in Molecular and Solid Fullerene Structures" at the Materials Research Society Spring meeting, San Francisco, CA.
5/92	Invited Talk on the "Structure and Dynamics of Large Fullerenes by First Principles Molecular Dynamics" at the Electrochemical Society Spring meeting, St. Louis, MO.
5/91	Mark Anderson Research Initiative Award (for best original research by a physics graduate student - "for novel and imaginative work on quantum molecular dynamics of semiconductor surfaces and Buckminsterfullerene molecules")
8/90 - 5/91	Regents Graduate Academic Scholarship
5/82	Physics Department Graduate Student Teaching Award (for best instruction by a graduate teaching assistant)
5/81	Sigma Pi Sigma (Physics Honor Society)

Ph.D. Dissertation

Title:	Applications of First Principles Quantum Molecular Dynamics: Semiconductor Surfaces and Fullerenes
Supervisor:	Professor Otto F. Sankey, Department of Physics and Astronomy, Arizona State University, Tempe, AZ
Completed:	Aug 1992

Research Experience

My research interest lies principally in first-principles simulations of semiconductor surfaces and of fullerenes, fullerene derivatives, and carbon nanotubes. I am especially interested in simulations in which molecular dynamics is useful. The first-principles molecular dynamics method in which I specialize is Quantum Molecular Dynamics (QMD), developed by Professor O.F. Sankey (Phys. Rev. B **40**, (1989) 3979) at Arizona State University. QMD is an approximate, non-self-consistent method which allows for the simulation of larger systems than is usually possible with plane-wave-based molecular dynamical methods, or the use of workstations rather than supercomputers. If more accuracy is required, I use a more recently developed, self-consistent, local-orbitals technique known as SIESTA (Phys. Rev. B **48**, 14646 (1993); **51** 1456 (1995)). When maximum accuracy is required, or when doing a static simulation involving only a small number of atoms, I use a fully self-consistent plane-wave method based on the work of M.P. Teter (Phys. Rev. B **40**, 12255 (1989)).

My interest in semiconductor surfaces began with my graduate work at Arizona State. In particular, I have studied the (100),(111), and (113) surfaces of silicon and the (100) and (111) surfaces of diamond carbon. We were the first to use first-principles molecular dynamical simulations to show that the (2x1) reconstruction of Si(111) can form directly from the bulk-terminated (111) surface without any significant energy barrier (Superlattices and Microstructures, **10**, 407 (1991)). I have also published first-principles simulations of aluminum deposited on the Si(100) surface, and participated in a more recent investigation of boron deposited on Si(100) (Phys. Rev. B**57**, 9745 (1998)).

My simulations of carbon fullerenes and nanotubes have been done in collaboration with Professors John Page, Michael O'Keeffe, Otto Sankey, and Jose Menéndez at Arizona State, Professor Jan Musfeldt at the University of Tennesse, Kati Kamarás at the Research Institute for Solid State Physics and Optics in Budapest, Hungary, and Virgina Long at Colby College in Waterville ME. Our work has included simulations of fullerenes with from 20 to 260 atoms. Our investigation of the energetics of large fullerenes was published in Science (**256**, 1792 (1992)). We were the first to suggest that fullerenes smaller than C_{60} might create solids that superconduct at a higher temperature than does doped C_{60} solid (Chemical Physics **176**, 61 (1993)). With the recent

isolations of C_{36} (Piskoti *et al.*, Nature **393**, 6687 (1998)) and of C_{20} (Prinzbach *et al.*, Nature **407**, 60 (2000)), it has become conceivable that this hypothesis might soon be tested. And, in a simulation that dramatically demonstrates the utility of first-principles molecular dynamics, we used QMD to predict the structure of the odd-mass fullerene derivative C_{119} (Chem. Phys. Lett. **228**, 485 (1994)). NMR and Raman spectroscopy have subsequently confirmed that our predicted structure is correct (Lebedkin *et al.*, J. Chem. Phys. **110**, 11768 (1999)). My most recent fullerene simulations have been of the Jahn Teller distortions of C_{60}^{-}, in collaboration with John Page and Virginia Long. Our talk at the 2004 APS March Meeting was entitled "Vibrational Study of the Jahn-Teller Distortion of C_{60}^{-} in $[AsPh_4]_2$ Cl C_{60}"

Finally, in addition to surfaces and fullerenes I am also interested in simulations of novel semiconducting solids. For example, silicon, germanium, and carbon clathrates (Phys. Rev. B**49**, 8048 (1994), Phil. Mag. Lett. **78** 21 (1998)) are found to be energetically competitive with the diamond forms, and the Si and Ge clathrates have bandgaps which are much wider than the respective diamond bandgaps. Si and Ge clathrates have now been synthesized, (see for example Gryko *et al.* Phys. Rev. B**57**, 4172 (1998)) and their thermoelectric properties are receiving considerable attention (see for example Nolas *et al.* Appl. Phys. Lett. **73** 178 (1998)). I have also simulated polybenzene, a three-coordinated carbon structure which is energetically comparable to solid C_{60} (Phys. Rev. Lett. **68**, 2325 (1992)) but which has not yet been synthesized.

Publications

1. "Far-Infrared Vibrational Properties of Linear C_{60} Polymers: a Comparison Between Neutral and Charged Materials", Z. -T. Zhu, J. L. Musfeldt, K. Kamarás, G. B. Adams, J. B. Page, V. C. Long, L.S. Kashevarova, A.V. Rakhmanina, V. A. Davydov, Y. Iwasa, W. E. Mayo, Phys. Rev. B **67**, 045409 (2003).
2. "Characterization of carbon nanotubes using Raman excitation profiles", M. Canonico, G.B. Adams, C. Poweleit, J. Menéndez, J.B. Page, G. Harris, H.P. van der Meulen, J.M. Calleja, and J. Rubio, Phys. Rev. B.**65** 201402 (2002).
3. "Far-infrared Vibrational Properties of the Tetragonal C_{60} Polymer", Z.-T. Zhu, J. L. Musfeldt, K. Kamarás, G. B. Adams, J. B. Page, V. A. Davydov, L. S. Kashevarova, and A. V. Rakhmanina, Phys. Rev. B.**65** 085413 (2002).
4. "Theoretical Studies of Raman Spectra for Planar Polymerized C_{60}", G.B. Adams and J.B. Page, Phys. Stat. Sol. B**226** 95 (2001).
5. "Far-infrared vibrational properties of high-pressure high-temperature C_{60} polymers and the C_{60} dimer", V.C. Long, J.L. Musfeldt, K. Kamarás, G.B. Adams, J.B. Page, Y. Iwasa, and W. E. Mayo, Phys. Rev. B**61** 13191 (2000).

6. "First-Principles Molecular Dynamical Studies of Polymerized C_{60}", G. B. Adams and J. B. Page, in *Fullerene Polymers and Fullerene-Polymer Composites*, edited by P. C. Eklund and A. M. Rao (Springer Verlag, Berlin) 2000, pp. 185 - 227.
7. "Quantum Molecular Dynamics Calculations and Experimental Raman Spectra Confirm the Proposed Structure of the Odd-Numbered Dimeric Fullerene C_{119}", S. Lebedkin, H. Rietschel, G.B. Adams, J.B. Page, W.E. Hull, F.H. Hennrich, H.-J. Eisler, M. M. Kappes, and W. Krätschmer, J. Chem. Phys. **110**, 11768 (1999).
8. "Duals of Frank-Kasper Structures as C, Si and Ge Clathrates: Energetics and Structure", M. O'Keeffe, G.B. Adams, and O.F. Sankey, Phil. Mag. Lett. **78** 21 (1998).
9. "First Principles Local-Orbital Study of the Boron-Induced Reconstruction of Si(001)", J. Fritsch, J.B. Page, and G.B. Adams, Phys. Rev. B**57**, 9745 (1998).
10. "Isotope Effect on the Raman Spectrum of the Pentagonal-Pinch Mode in C_{60}", S. Guha, J. Menéndez, J.B. Page, and G.B. Adams, Phys. Rev. B**56**, 15431 (1997).
11. "Empirical Bond Polarizability Model for Fullerenes", S. Guha, J. Menéndez, J.B. Page, and G.B. Adams, Phys. Rev. B**53**, 13106 (1996).
12. "Neutron Diffraction and Structural Models of RbC_{60} Phases", J.R. Fox, G.P. Lopinski, J.S. Lannin, G.B. Adams, J.B. Page, and J.E. Fischer, Chem. Phys. Lett. **249**, 195 (1996).
13. "A First Principles Molecular Dynamics Study of the Fullerene Derivative C_{119}", G.B. Adams, J.B. Page, M. O'Keeffe, and O.F. Sankey, Chem. Phys. Lett. **228**, 485 (1994).
14. "Polymerized C_{60} Studied by First Principles Molecular Dynamics", G.B. Adams, J.B. Page, O.F. Sankey, and M. O'Keeffe, Phys. Rev. B**50**, 17471 (1994).
15. "Van Der Waals Surface Areas and Volumes of Fullerenes", G.B. Adams, M. O'Keeffe, and R.S. Ruoff, J. Phys. Chem. **98**, 9465 (1994).
16. "Isotopically Resolved Raman Spectra of C_{60}", S. Guha, J. Menéndez, J.B. Page, G.B. Adams, G.S. Spencer, J.P. Lehman, P. Giannozzi, and S. Baroni, Phys. Rev. Lett. **72**, 3359 (1994).
17. "Wide-Bandgap Si in Open Four-Coordinated Clathrate Structures", G.B. Adams, M. O'Keeffe, A.A. Demkov, O.F. Sankey, and Y.M. Huang, Phys. Rev. B**49**, 8048 (1994).
18. "Jahn-Teller Distortions in Solid C_{20} and Other Fullerene Structures", G.B. Adams, O.F. Sankey, J.B. Page, and M. O'Keeffe, Chemical Physics **176**, 61 (1993).
19. "Energetics of Large Fullerenes: Balls, Tubes, and Capsules", G. B. Adams, O.F. Sankey, J.B. Page, M. O'Keeffe, and David A. Drabold, Science **256**, 1792 (1992).
20. "Polybenzene, a Predicted New Low Energy Form of Carbon", G.B. Adams, M. O'Keeffe, O.F. Sankey, and J.B. Page, Materials Research Society Symposium Proceedings, Vol. 270, Novel Forms of Carbon, edited by C. L. Renschler, J. J. Pouch and D. M. Cox, 1993, pp. 103-108.
21. "Predicted New Low Energy Forms of Carbon", M. O'Keeffe, G.B. Adams, and O.F. Sankey, Phys. Rev. Lett. **68**, 2325 (1992).

22. "Applications of *Ab Initio* Quantum Molecular Dynamical Relaxation: Silicon(111)-5×5 Surface Reconstruction and Aluminum Deposited on Silicon(100)", G.B. Adams and O.F. Sankey, Jour. Vac. Sci. Tech. A **10**, 2046 (1992).
23. "*Ab Initio* Molecular Dynamical Relaxation Applied to the Silicon(111)-5x5 Surface Reconstruction", G.B. Adams and O.F. Sankey, Phys. Rev. Lett. **67**, 867 (1991).
24. "First-Principles Quantum-Molecular-Dynamics Study of the Vibrations of Icosahedral C_{60}", G.B. Adams, J.B. Page, O.F.Sankey, K. Sinha, J. Menéndez, and D.R. Huffman, Phys. Rev. B (RC) **44**, 4052 (1991).
25. "First-Principles Electronic Structure Calculations with Molecular Dynamics Made Easy", O.F. Sankey, G.B. Adams, X. Weng, J.D. Dow, Y.M. Huang, J.C.H. Spence, D.A. Drabold, Wei-Min Hu, R.P. Wang, S. Klemm, and P.A. Fedders, Superlattices and Microstructures, **10**, 407 (1991).
26. "The Influence of Internal Surfaces on the (2x1) Shuffle and Glide Cleavage Reconstructions of Si(111)", Y.M. Huang, J.C.H. Spence, O.F. Sankey, and G.B. Adams, Surface Science, **256**, 344 (1991).
27. "Superperiodic Features Observed on Graphite under Solution with Scanning Tunneling Microscopy", P.I. Oden, T. Thundat, L. Nagahara, S. Lindsay, G.B. Adams, and O.F. Sankey, Surface Science, **254**, L454 (1991).

Submissions and Papers in Preparation

1. "Jahn-Teller distortion of C_{60}^- in $(Ph_4As)_2ClC_{60}$: C_{2h} versus C_i", V.C. Long, E.C. Schundler, G.B. Adams, J.B. Page, W. Bietsch, and I. Bauer, submitted to Phys. Rev. B.

Conference Abstracts

1. "Vibrational Study of the Jahn-Teller Distortion of C_{60}^- in $[AsPh_4]_2$ Cl C_{60}", V.C. Long, E.C. Schundler, G.B. Adams, J.B. Page, W. Bietsch, and I. Bauer, 2004 March Meeting of the American Physical Society, Montreal, Quebec, Canada, March 2004.
2. "Calculated Raman Spectra for the Odd-Numbered Fullerene C_{139}", G.B.Adams and J.B.Page, 2003 March Meeting of the American Physical Society, Austin, TX, March 2003.
3. "The Evolution of I_h C_{60} Vibrational Modes in Planar Polymerized C_{60}", G.B.Adams and J.B.Page, 2001 March Meeting of the American Physical Society, Seattle, WA, March 2001.
4. "Two-Dimensional Polymerization of C_{60} Simulated with First-Principles Molecular Dynamics", G.B.Adams and J.B.Page, 1999 March Meeting of the American Physical Society, Atlanta, GA, March 1999.
5. "Polymerization in RbC_{60} and KC_{60} as Simulated with First-Principles Molecular Dynamics", G.B.Adams and J.B.Page, 1997 March Meeting of the American Physical Society, Kansas City, MO, March 1997.
6. "First-Principles Calculations of Infrared Absorption Strengths for Large Fullerenes", G.B.Adams, J.B.Page, and O.F.Sankey, 1995 March Meeting of the American Physical Society, San Jose, CA, March 1995.
7. "Local-Orbital-Based Quantum Molecular Dynamics Simulations of C_{60} on Silicon Surfaces", G.B.Adams, M. O'Keeffe, J.B.Page, and O.F.Sankey, Invited Talk, 185th Meeting of the Electrochemical Society, San Francisco, CA, May 1994.

8. "A First Principles Study of Polymeric Joinings of Fullerene Molecules", G.B.Adams, J.B.Page, M. O'Keeffe, and O.F.Sankey, 1994 March Meeting of the American Physical Society, Pittsburgh, PA, March 1994.
9. "A First Principles Molecular Dynamical Study of Polymerized C_{60} and of C_{119}", G.B.Adams, J.B.Page, M. O'Keeffe, and O.F.Sankey, Invited Talk, 184th Meeting of the Electrochemical Society, New Orleans, LA, October 1993.
10. "Jahn-Teller Interactions in Molecular and Solid Fullerene Structures", G.B. Adams, M. O'Keeffe, O.F. Sankey, and J.B. Page, Invited Talk, Spring Meeting of the Materials Research Society, San Francisco, CA, April 1993.
11. "Jahn-Teller Interactions in Molecular and Solid Fullerenes", G.B. Adams, M. O'Keeffe, O.F. Sankey, and J.B. Page, 1993 March Meeting of the American Physical Society, Seattle, WA, March 1993.
12. "Structure and Dynamics of Large Fullerenes by First Principles Molecular Dynamics", G.B. Adams, J.B. Page, O.F.Sankey, K. Sinha, J. Menéndez, and M. O'Keeffe, Invited Talk, 182nd Meeting of the Electrochemical Society, St. Louis, MO, May 1992.
13. "Predicted New Low Energy Forms of Carbon", G.B. Adams, M. O'Keeffe, and O.F. Sankey, Spring Meeting of the Materials Research Society, San Francisco, CA, April 1992.
14. "Structure and Dynamical Properties of Fullerenes and Other Novel Forms of Carbon Determined by First Principles Molecular Dynamics", G.B. Adams, J.B. Page, O.F. Sankey, and M. O'Keeffe, Spring Meeting of the Materials Research Society, San Francisco, CA April 1992.
15. "Pseudo-Atomic-Orbital Based First Principles Molecular Dynamics Applied to Structural Determination and Dynamical Properties of Surfaces and Novel Materials", O.F. Sankey, G.B. Adams, and J.B. Page, Spring Meeting of the Materials Research Society, San Francisco, CA April 1992.
16. "Structure and Dynamical Properties of Fullerenes and Other Novel Forms of Carbon by First Principles Molecular Dynamics", G.B.Adams, J.B.Page, O.F.Sankey, K.Sinha, J.Menéndez, and M. O'Keeffe, 1992 March Meeting of the American Physical Society, Indianapolis, IND, March 1992.
17. "*Ab Initio* Quantum Molecular Dynamics of Si Surfaces: (111)-5x5 and Other Reconstructions", O.F. Sankey and G.B. Adams, 38th Annual Symposium and Topical Conferences of the American Vacuum Society, Seattle, WA, November 1991.
18. "First Principles Quantum Molecular Dynamics Applied to C_{60}, C_{70}, and Higher Mass Carbon Cages", G.B. Adams, J.B. Page, O.F. Sankey, K. Sinha, J. Menéndez, and D.R. Huffman, 180th Meeting of the Electrochemical Society, Special Session on "FULLERENES: Chemistry, Physics, and New Directions", Phoenix, AZ, October 1991.
19. "Theoretical and Experimental Raman Study of the Buckyball C_{60}", G.B. Adams, J.B. Page, O.F. Sankey, K. Sinha, J. Menéndez, and D.R. Huffman, 1991 March Meeting of the American Physical Society, Postdeadline Session on Fullerenes, Cincinnati, OH, March 1991.
20. "First Principles Quantum Molecular Dynamics with the Silicon(111)-5x5 Reconstructed Surface", G.B. Adams and O.F. Sankey, 1991 March Meeting of the American Physical Society, Cincinnati, OH, March 1991.

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