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Personal

Born May 10, 1948
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Education

B.S. Physics, Vanderbilt University, 1969.
M.S. Physics, University of North Carolina, 1970.
Ph.D. Chemical Physics, Columbia University, 1978.

Positions Held

Member of Technical Staff, Bell Laboratories/Bellcore, 1981-85.
Senior Research Scientist, United Technologies Research Center, 1985-1994.
Senior Research Scientist, Gaussian, Inc., 1994-2008.
Research Professor, University of Connecticut, 2008-present.

Students Mentored

Sandipan Banerjee, Ph.D, University of Connecticut, 2013.
Jason Byrd, Ph.D, University of Connecticut, 2013.

Publications (18 at UConn)

1. S. Green, J. A. Montgomery, Jr., and P. Thaddeus, "Tentative Identification of U93.174 as the Molecular Ion NNH^+ ", *Ap. J. (Letters)* **193**, L89 (1974).
2. B. J. Berne and J. A. Montgomery, Jr., "The Coupling Between Translational and Rotational Motions", *Mol. Phys.* **32**, 363 (1976).
3. J. A. Montgomery, Jr. and B. J. Berne, "A Viscoelastic Theory of the Angular Velocity Correlation Function", *J. Chem. Phys.* **66**, 2161 (1977).
4. J. A. Montgomery, Jr. and B. J. Berne, "A Hydrodynamic Theory of the Angular Velocity Correlation Function with Arbitrary Slip Boundary Conditions", *J. Chem. Phys.* **66**, 2770 (1977).

5. J. A. Montgomery, Jr. and B. J. Berne, "Molecular Hydrodynamics of the Partially Rough Sphere Fluid", *J. Chem. Phys.* **67**, 4580 (1977).
6. J. M. Deutch, P. G. Wolynes, J. A. Montgomery, Jr. and B. J. Berne, "The Effects of Hydrodynamic Interactions on Translational and Rotational Relaxation", *J. Chem. Phys.* **67**, 4589 (1977).
7. J. A. Montgomery, Jr. and B. J. Berne, "On the Effects of Translation-Rotation Coupling on Hydrodynamic Rotation Tensors", *J. Chem. Phys.* **67**, 5971 (1977).
8. J. A. Montgomery, Jr., D. Chandler, and B. J. Berne, "Trajectory Analysis of a Kinetic Theory for Isomerization Dynamics in Condensed Phases", *J. Chem. Phys.* **70**, 4056 (1977).
9. C. E. Dykstra and J. A. Montgomery, Jr., "The Equilibrium Structure and Rotational Constant of HCC^+ ", *J. Chem. Phys.* **71**, 1380 (1979).
10. J. A. Montgomery, Jr., S. L. Holmgren, and D. Chandler, "Stochastic Molecular Dynamics Study of *trans-gauche* Isomerization Dynamics in Condensed Phases", *J. Chem. Phys.* **73**, 3688 (1980).
11. J. A. Montgomery, Jr. and H. H. Michels, "On the Stability of H_4 in C_{3v} Symmetry", *J. Chem. Phys.* **86**, 5882 (1987).
12. J. A. Montgomery, Jr. and H. H. Michels, "On the Structure of the Ground State of H_6^+ ", *J. Chem. Phys.* **87**, 771 (1987).
13. H. H. Michels and J. A. Montgomery, Jr., "The Electronic Structure and Stability of the H_3^- Anion", *Chem. Phys. Lett.* **139**, 535 (1987).
14. R. A. Kuharski, D. Chandler, J. A. Montgomery, Jr., F. Rabii, and S. J. Singer, "Stochastic Molecular Dynamics Study of Cyclohexane Isomerization", *J. Phys. Chem.* **92**, 3261 (1988).
15. H. H. Michels and J. A. Montgomery, Jr., "The Electronic Structure and Stability of Asymmetric Dinitrogen Dioxide ($\alpha\text{-N}_2\text{O}_2$)", *J. Chem. Phys.* **88**, 7248 (1988).
16. J. A. Montgomery, Jr. and H. H. Michels, "Reply to "Comment: On the Stability of H_4 in C_{3v} Symmetry", *J. Chem. Phys.* **89**, 3929 (1988).
17. J. A. Montgomery, Jr., G. A. Petersson, and N. Matsunaga, "On the Helium Pair Potential", *Chem. Phys. Lett.* **155**, 413 (1989).
18. J. A. Montgomery, Jr., H. H. Michels, O. F. Güner, and K. Lammertsma, "The Structure and Bonding of Li_3H Ion-Pair States", *Chem. Phys. Lett.* **161**, 291 (1989).
19. J. A. Montgomery, Jr. and G. A. Petersson, "On the C-H Bond Dissociation Energy of Acetylene", *Chem. Phys. Lett.* **168**, 75 (1990).
20. H. H. Michels and J. A. Montgomery, Jr., "The Electronic Structure and Stability of NF_5 and PF_5 ", *J. Chem. Phys.* **93**, 1805 (1990).

21. J. A. Montgomery, Jr., G. A. Petersson, M. A. Al-Laham, and J. Mantzaris, "On the Dissociation Energy of NF ($X^3\Sigma^-$)", *Chem. Phys. Lett.* **169**, 497 (1990).
22. G. A. Petersson, T. G. Tensfeldt, and J. A. Montgomery, Jr., "A Complete Basis Set Model Chemistry III. The CBS-QCI Family of Methods", *J. Chem. Phys.* **94**, 6091 (1991).
23. M. W. Schmidt, K. A. Nguyen, M. S. Gordon, and J. A. Montgomery, Jr., "Systematic Survey of Cyclic Silicon-Oxygen Compounds", *J. Am. Chem. Soc.* **113**, 5998 (1991).
24. G. A. Petersson, T. G. Tensfeldt, and J. A. Montgomery, Jr., "Vinylidene and the Hammond Postulate", *J. Am. Chem. Soc.* **114**, 6133 (1992).
25. K. A. Nguyen, M. S. Gordon, J. A. Montgomery, Jr., H. H. Michels, and D. R. Yarkony, "Theoretical Studies of Spin-Forbidden Radiationless Decay in Polyatomic Systems II: Radiationless Decay of $\alpha\text{-N}_2\text{O}_2$ ", *J. Chem. Phys.* **98**, 3845 (1993).
26. J. M. Van Doren, A. A. Viggiano, R. A. Morris, A. E. Stevens Miller, T. M. Miller, J. F. Paulson, C. A. Deakyne, H. H. Michels and J. A. Montgomery, Jr., "Experimental and Theoretical Study of the Reaction of HO^- with NO", *J. Chem. Phys.* **98**, 7940 (1993).
27. H. H. Michels and J. A. Montgomery, Jr., "On the Structure and Thermochemistry of Hydrogen Dinitramide", *J. Phys. Chem.* **97**, 6602 (1993).
28. M. W. Schmidt, K. K. Baldrige, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. H. Jensen, S. Koseki, N. Matsunaga, K. A. Nguyen, S. Su, T. L. Windus, M. Dupuis, and J. A. Montgomery, Jr., "The General Atomic and Molecular Electronic Structure System", *J. Comp. Chem.* **14**, 1347 (1993).
29. J. A. Montgomery, Jr. and H. H. Michels, "The Structure and Stability of Trinitramide", *J. Phys. Chem.* **97**, 6674 (1993).
30. J. A. Montgomery, Jr., H. H. Michels, and J. S. Francisco, "Ab initio calculation of the Heats of Formation of CF_3OH and CF_2O ", *Chem. Phys. Lett.* **220**, 391 (1994).
31. D. J. Benard, E. Boehmer, H. H. Michels and J. A. Montgomery, Jr., "Energy Transfer from Metastable NF to Boron Hydride", *J. Phys. Chem.* **98**, 8952 (1994).
32. K. A. Nguyen, M. S. Gordon, J. A. Montgomery, Jr., and H. H. Michels, "Structures, Bonding, and Energetics of N_2O_2 Isomers", *J. Phys. Chem.* **98**, 10072 (1994).
33. J. A. Montgomery, Jr., J. W. Ochterski, and G. A. Petersson, "A complete basis set model chemistry IV. An improved CBS-QCI/APNO method", *J. Chem. Phys.* **101**, 5900 (1994).
34. H. H. Michels, J. A. Montgomery, Jr., K. O. Christie, and D. A. Dixon, "Theoretical Prediction of the Structures and Stabilities of Azidamines", *J. Phys. Chem.* **99**, 187 (1995).
35. J. W. Ochterski, G. A. Petersson, and J. A. Montgomery, Jr., "A complete basis set model chemistry V. Extensions to six or more heavy atoms", *J. Chem. Phys.* **104**, 2598 (1996).

36. A. A. Viggiano, R. A. Morris, T. M. Miller, J. F. Friedman, M. Menedez-Barreto, J. F. Paulson, H. H. Michels, R. H. Hobbs, and J. A. Montgomery, Jr., "Reaction on the $O^- + CH_4$ potential energy surface: Dependence on translational and internal energy and on isotopic composition, 93-1313 K", *J. Chem. Phys.* **106**, 8455 (1997).
37. D. K. Malick, G. A. Petersson, and J. A. Montgomery, Jr., "Transition states for chemical reactions I. Geometry and classical barrier height", *J. Chem. Phys.* **108**, 5704 (1998).
38. J. A. Montgomery, Jr., M. J. Frisch, J. W. Ochterski, G. A. Petersson, K. Raghavachari, and V. G. Zakrzewski, Comment on "Assessment of complete basis set methods for calculation of enthalpies of formation" [*J. Chem. Phys.* **108**, 692 (1998)], *J. Chem. Phys.* **109**, 6505 (1998).
39. G. A. Petersson, D. K. Malick, W. G. Wilson, J. W. Ochterski, J. A. Montgomery, Jr., and M. J. Frisch, "Calibration and comparison of the Gaussian-2, complete basis set, and density functional methods for computational thermochemistry", *J. Chem. Phys.* **109**, 10570 (1998).
40. J. A. Montgomery, Jr., M. J. Frisch, J. W. Ochterski, and G. A. Petersson, "A complete basis set model chemistry VI. Use of density functional geometries and frequencies", *J. Chem. Phys.* **110**, 2822 (1999).
41. J. A. Montgomery, Jr., M. J. Frisch, J. W. Ochterski, and G. A. Petersson, "A complete basis set model chemistry VII. Use of the minimum population localization method", *J. Chem. Phys.* **112**, 6532 (2000).
42. A. J. Austin, M. J. Frisch, J. A. Montgomery, Jr., and G. A. Petersson, "An overlap criterion for selection of core orbitals", *Theor. Chem. Acc.* **107**, 180 (2002).
43. G. A. Petersson, S. Zhong, J. A. Montgomery, Jr., and M. J. Frisch, "On the optimization of Gaussian basis sets", *J. Chem. Phys.* **118**, 1101 (2003).
44. T. Vreven, K. S. Byun, I. Komáromi, S. Dapprich, J. A. Montgomery, Jr., K. Morokuma, and M. J. Frisch, "Combining Quantum Mechanics Methods with Molecular Mechanics Methods in ONIOM", *J. Chem. Theory Comput.* **2**, 825 (2006).
45. G. P. F. Wood, L. Radom, G. A. Petersson, E. C. Barnes, M. J. Frisch, and J. A. Montgomery, Jr., "A restricted-open-shell complete-basis-set model chemistry", *J. Chem. Phys.* **125**, 094106 (2006).
46. J. N. Byrd, J. A. Montgomery, Jr., H. H. Michels, and R. Côté, "Potential energy surface of the $1^2A'$ $Li_2 + Li$ doublet ground state", *Int. J. Quantum Chem.* **109**, 3112 (2009).
47. J. N. Byrd, J. A. Montgomery, Jr., H. H. Michels, and R. Côté, "Electronic structure of the $Li_2 [X^1\Sigma_g^+] + Li [^2P]$ excited $^2A''$ surface", *Int. J. Quantum Chem.* **109**, 3626 (2009).
48. E. C. Barnes, G. A. Petersson, J. A. Montgomery, Jr., M. J. Frisch, and J. M. L. Martin, "Unrestricted Coupled Cluster and Brueckner Doubles Variations of W1 Theory", *J. Chem. Theory Comput.* **5**, 2687 (2009).
49. G. B. Churchill, J. P. Dombrowski, L. Ma, K. Swana, R. K. Bohn, J. A. Montgomery, Jr., "Microwave spectroscopy and conformations of 2-methylbutane and 2,3-dimethylbutane", *J. Mol. Struct.* **978**, 11 (2010).

50. J. A. Fournier, R. K. Bohn, J. A. Montgomery, Jr., and M. Onda, "The Helical C_2 Structure of Perfluoropentane and the C_{2v} Structure of Perfluoropropane", *J. Phys. Chem. A* **114**, 1118 (2010)
51. W. T. Zemke, J. N. Byrd, H. H. Michels, J. A. Montgomery, Jr. and W. C. Stwalley, "Long Range Intermolecular Interactions Between the Alkali Diatomics Na_2 , K_2 and NaK ", *J. Chem. Phys.*, **132**, 244305 (2010)
52. J. N. Byrd, J. A. Montgomery, Jr. and R. Côté, "Structure and thermochemistry of K_2Rb , KRb_2 and K_2Rb_2 ", *Phys. Rev. A* **82**, 010502(R) (2010)
53. S. Banerjee, J. N. Byrd, R. Côté, H. H. Michels, and J. A. Montgomery, Jr, "Ab initio potential curves for the $X^2\Sigma_u^+$ and $B^2\Sigma_g^+$ states of Be_2^+ : Existence of a double minimum", *Chem. Phys. Lett.* **496**, 208 (2010)
54. J. N. Byrd, R. Côté and J. A. Montgomery, Jr. "Long range interactions between like homonuclear alkali metal diatoms," *J. Chem. Phys.* **135**, 244307 (2011)
55. J. N. Byrd, H. H. Michels, R. Côté, J. A. Montgomery, Jr. and W. C. Stwalley, "Structure, Energetics and Reactions of Alkali Tetramers," *J. Chem. Phys.* **136**, 014306 (2012)
56. J. N. Byrd, H. H. Michels, J. A. Montgomery, Jr. and R. Côté, "Long-range three-body atom-diatom potential for doublet Li_3 ", *Chem. Phys. Lett.* **529**, 23 (2012)
57. S. Banerjee, J. A. Montgomery, Jr, J. N. Byrd, H. H. Michels and R. Côté, "Ab initio potential curves for the $X^2\Sigma_u^+$, $A^2\Pi_u$ and $B^2\Sigma_g^+$ states of Ca_2^+ ", *Chem. Phys. Lett.* **542**, 138 (2012)
58. J. N. Byrd, J. A. Montgomery, Jr. and R. Côté, "Controllable binding of polar molecules and meta-stable of 1-D dipolar gases with attractive dipole forces", *Phys. Rev. Lett.* **109**, 083003 (2012)
59. S. Banerjee, J. A. Montgomery, Jr, and J. A. Gascon. "A QM/MM approach to the study of monolayer-protected gold clusters", *J. Mater. Sci.* **47**, 7686 (2012)
60. J. N. Byrd, J. A. Montgomery, Jr. and R. Côté, "Long range forces between polar alkali diatoms aligned by external electric fields", *Phys. Rev. A* **86**, 032711 (2012)
61. J. N. Byrd, H. H. Michels, J. A. Montgomery, Jr. and R. Côté, "Associative detachment of rubidium hydroxide", *Phys. Rev. A* **88**, 032710 (2013)
62. J. N. Byrd, R. J. Bartlett and John A. Montgomery, Jr., "At what chain length do unbranched alkanes prefer folded conformations?", *J. Phys. Chem. A* **118**, 1706 (2014)
63. W. W. Smith, D. S. Goodman, I. Sivarajah, J. E. Wells, S. Banerjee, R. Côté, H. H. Michels, J. A. Montgomery, Jr. and F. A. Narducci, "Experiments with an ion-neutral hybrid trap: Cold charge-exchange collisions", *Appl. Phys. B* **114**, 75 (2014)
64. R. K. Bohn, J. A. Montgomery, Jr., H. H. Michels and J. A. Fournier, "Second Moments and Microwave Spectroscopy", *J. Mol. Spec.* (manuscript in preparation).