

Publications of William A. Lester, Jr.

Books

1. *Proceedings of the Conference on Potential Energy Surfaces in Chemistry*, ed. W. A. Lester, Jr., Research Library, IBM Research Laboratory (San Jose, California 95193) (1971).
2. B. L. Hammond, W. A. Lester, Jr., and P. J. Reynolds, *Monte Carlo Methods in Ab Initio Quantum Chemistry*, World Scientific (Singapore) (1994).
3. *Recent Advances in Quantum Monte Carlo Methods*, ed., W. A. Lester, Jr., World Scientific Publishing (Singapore) (1997).
4. *Proceedings of the First International Workshop on Contemporary Problems in Mathematical Physics*, eds. J. Govaerts, M. N. Hounkonnou, and W. A. Lester, Jr., World Scientific Publishing (Singapore) (2000).
5. *Recent Advances in Quantum Monte Carlo – Part II*, eds. S. Rothstein, W. A. Lester, Jr., and S. Tanaka, World Scientific Publishing (Singapore) (2002).

Abstracts, Articles, and Chapters

1. W. A. Lester, Jr. and M. Krauss, “Gaussian Correlation Functions: Two Electron Systems,” *J. Chem. Phys.* **41**, 1407 (1964).
2. W. A. Lester, Jr. and M. Krauss, “Some Aspects of the Coulomb Hole of the Ground State of H_3^+ ” *J. Chem. Phys.* **44**, 207 (1966).
3. W. A. Lester, Jr. and R. B. Bernstein, “Structural Features of the S-Matrix for the Rotational Excitation of Homonuclear Diatomic Molecules by Atom Impact: Close-Coupled versus Approximate Computations,” *Chem. Phys. Lett.* **1**, 207 (1967).
4. B. R. Johnson, D. Secrest, W. A. Lester, Jr., and R. B. Bernstein, “A Validation of the Method of Amplitude Density Functions in Computing the S-Matrix for a Scattering Problem,” *Chem. Phys. Lett.* **1**, 396 (1967).
5. W. A. Lester, Jr. and R. B. Bernstein, “Computational Procedure for the Close-Coupled Rotational Excitation Problem: Scattering of Diatomic Molecules by Atoms,” *J. Chem. Phys.* **48**, 4896 (1968).
6. W. A. Lester, Jr., “DeVogelaere’s Method for the Numerical Integration of Second-Order Differential Equations without Explicit First Derivatives: Application to Coupled Equations Arising from the Schrödinger Equation,” *J. Comput. Phys.* **3**, 322 (1968).
7. W. A. Lester, Jr. and M. Krauss, “Interaction Potential between Li and HF,” *J. Chem. Phys.* **52**, 4775 (1970).
8. W. A. Lester, Jr. and R. B. Bernstein, “Statistical Analysis of Transition Probability Matrices in the Strong Coupled Rotational Excitation Problem,” *J. Chem. Phys.* **53**, 11 (1970).
9. W. A. Lester, Jr., “Interaction Potential between Li^+ and H_2 . I. Region Appropriate for Rotational Excitation,” *J. Chem. Phys.* **53**, 1511 (1970).
10. W. A. Lester, Jr., “Analytical Expression for the Interaction Potential between Li and HF,” *J. Chem. Phys.* **53**, 1611 (1970).
11. W. A. Lester, Jr., “Interaction Potential between Li^+ and HD: Region for Rotational Excitation Cross Sections,” *IBM J. Res. Dev.* **15**, 222 (1971).

12. W. A. Lester, Jr., “Interaction Potential between Li^+ and H_2 . II. Region Appropriate for Rotational Vibrational Excitation,” *J. Chem. Phys.* **54**, 3171 (1971).
13. W. A. Lester, Jr., “Potential Surfaces for Internal Energy Transfer” in *Proceedings of the Conference on Potential Energy Surfaces in Chemistry*, IBM Research Laboratory (San Jose, California 95193), p 113 (1971).
14. W. A. Lester, Jr., “Thermal Energy $Li^+ - H_2$ Collisions,” Abstracts of the VII International Conference on the Physics of Electronic and Atomic Collisions, North Holland (Amsterdam), p 247 (1971).
15. W. A. Lester, Jr., “Calculation of Cross Sections for Rotational Excitation of Diatomic Molecules by Heavy Particle Impact: Solution of the Close-Coupled Equations,” *Methods Comput. Phys.* **10**, 211 (1971).
16. W. A. Lester, Jr. and J. Schaefer, “Rotational Excitation of H_2 by Li^+ Collisions below the First Vibrational Threshold,” *Bull. Am. Phys. Soc.* **17**, 1142 (1972).
17. J. Schaefer and W. A. Lester, Jr., “Vibration-Rotation Excitation of H_2 by Li^+ Collisions,” *Bull. Am. Phys. Soc.* **17**, 1142 (1972).
18. W. A. Lester, Jr., “The Accurate Calculation of Cross-Sections for Non-Reactive Molecular Collisions” in *Computing as a Language of Physics*, International Atomic Energy Agency (Vienna, Austria), p 375 (1972).
19. J. Schaefer and W. A. Lester, Jr., “Effect of Rotation on Vibrational Excitation of H_2 by Li^+ Impact,” *Chem. Phys. Lett.* **20**, 575 (1973).
20. J. Schaefer and W. A. Lester, Jr., “Cross Sections for Vibrational Excitation of H_2 by Li^+ Impact,” Abstracts of the VIII International Conference on the Physics of Electronic and Atomic Collisions, Institute of Physics (Beograd, Yugoslavia), p 91 (1973).
21. W. A. Lester, Jr. and J. Schaefer, “Coupled-Channel Calculations of Rotational Excitation of H_2 and Li^+ Collisions,” Abstracts of the VIII International Conference on the Physics of Electronic and Atomic Collisions, Institute of Physics (Beograd, Yugoslavia), p 92 (1973).
22. W. A. Lester, Jr. and J. Schaefer, “Coupled Channel Study of Rotational Excitation of H_2 by Li^+ Collisions,” *J. Chem. Phys.* **59**, 3676 (1973).
23. J. Schaefer, W. A. Lester, Jr., D. Kouri, and C. A. Wells, “Anharmonicity in Rotational and Vibrational Excitation of H_2 by Li^+ Collisions,” *Chem. Phys. Lett.* **24**, 185 (1974).
24. W. A. Lester, Jr. and J. Schaefer, “Rotational Transitions in H_2 by Li^+ Collisions at $E_{cm} = 0.6$ eV: Comparison with Experiment,” *Bull. Am. Phys. Soc.* **19**, 261 (1974).
25. A. C. Yates and W. A. Lester, Jr., “A New H_3 Potential Energy Surface and Its Implications for Chemical Reaction,” *Chem. Phys. Lett.* **24**, 305 (1974).
26. W. A. Lester, Jr. and J. Schaefer, “Rotational Transitions in H_2 by Li^+ Collisions at $E_{cm} = 0.6$ eV; Comparison with Experiment,” *J. Chem. Phys.* **60**, 1672 (1974).
27. B. J. Garrison, H. F. Schaefer, III, and W. A. Lester, Jr., “Molecular Properties of Excited Electronic States: The $\tilde{\alpha}^3A$ ” and $\tilde{\Lambda}^1A$ ” States of Formaldehyde,” *J. Chem. Phys.* **61**, 3039 (1974).

28. J. Schaefer and W. A. Lester, Jr., "Theoretical Study of Inelastic Scattering of H₂ and Li⁺ on SCF and CI Potential Energy Surfaces," *J. Chem. Phys.* 62, 1913 (1975).
29. W. A. Lester, Jr., "Coupled-Channel Studies of Rotational and Vibrational Energy Transfer by Collision," *Adv. Quantum Chem.* 9, 199 (1975).
30. B. J. Garrison and W. A. Lester, Jr., "Cross Sections for Rotational Excitation of H₂CO by He Impact at Low Energies," Abstracts of the IXth International Conference on the Physics of Electronic and Atomic Collisions, University of (Washington Press, Seattle, Washington), p 55 (1975).
31. S. Green, B. J. Garrison, and W. A. Lester, Jr., "Hartree-Fock and Gordon-Kim Interaction Potentials for Scattering of Closed-Shell Molecules by Atoms: (H₂CO, He) and (H₂, Li⁺)," *J. Chem. Phys.* 63, 1154 (1975).
32. B. J. Garrison, W. A. Lester, Jr., and H. F. Schaefer, III, "A Hartree-Fock Interaction Potential between a Rigid Asymmetric Top and a Spherical Atom: (H₂CO, He)," *J. Chem. Phys.* 63, 1449 (1975).
33. B. J. Garrison, W. A. Lester, Jr., W. H. Miller, and S. Green, "Cooling of the 6-cm and 2-cm Doublets of Interstellar H₂CO by Collision: An Accurate Quantum-Mechanical Calculation," *Astrophys. J.* 200, L175 (1975).
34. B. J. Garrison, W. A. Lester, Jr., P. Siegbahn, and H. F. Schaefer, III, "Effect of Electron Correlation on the H₂CO-He Interaction Potential," *J. Chem. Phys.* 63, 4167 (1975).
35. F. Rebentrost and W. A. Lester, Jr., "Nonadiabatic Effects in the Collision of F(²P) with H₂(¹ Σ_g^+). I. SCF Interaction Potentials for the ¹A', ²A' and ²A'' States in the Reactant Region," *J. Chem. Phys.* 63, 3737 (1975).
36. F. Rebentrost and W. A. Lester, Jr., "Nonadiabatic Effects in the Collision of F(²P) with H₂(¹ Σ_g^+). II. Born-Oppenheimer and Angular Momentum Coupling in Adiabatic and Diabatic Representations," *J. Chem. Phys.* 64, 3879 (1976).
37. F. Rebentrost and W. A. Lester, Jr., "Resonant Electronic-to-Rotational Energy Transfer. Quenching of F(²P_{1/2}) by H₂(j=0)," *J. Chem. Phys.* 64, 4223 (1976).
38. W. A. Lester, Jr., "Computer in Chemistry" in *A Century of Chemistry*, American Chemical Society (Washington, DC), p 286 (1976).
39. A. S. Dickenson, D. J. Kouri, C. A. Wells, and W. A. Lester, Jr., "An Eigenphase Study of the Resonances in the Rotational Excitation of H₂ by Li⁺ Immediately above the j = 2 Threshold," *J. Chem. Phys.* 65, 1501 (1976).
40. W. A. Lester, Jr., "The N Coupled-Channel Problem" in *Modern Theoretical Chemistry*, Plenum Press (New York), Vol. 3, p 1 (1976).
41. B. J. Garrison, W. A. Lester, Jr., and W. H. Miller, "Coupled-Channel Study of Rotational Excitation of a Rigid Asymmetric Top by Atom Impact: (H₂CO, He) at Interstellar Temperatures," *J. Chem. Phys.* 65, 2193 (1976).
42. R. E. Howard, A. C. Yates, and W. A. Lester, Jr., "Collinear Classical Dynamics on a Chemically Accurate H + H₂ Potential Energy Surface," *J. Chem. Phys.* 66, 1960 (1977).
43. B. J. Garrison and W. A. Lester, Jr., "Coupled States Cross Sections for Rotational Excitation of H₂CO by He Impact at Interstellar Temperatures," *J. Chem. Phys.* 66, 531 (1977).
44. A. W. Raczkowski and W. A. Lester, Jr., "Extension of a He-H₂ Potential Energy Surface," *Chem. Phys. Lett.* 47, 45 (1977).
45. F. Rebentrost and W. A. Lester, Jr., "Nonadiabatic Effects in the Collision of F(²P) with H₂(¹ Σ_g^+). III. Scattering Theory and Coupled-Channel Computations," *J. Chem. Phys.* 67, 3367 (1977).
46. F. Rebentrost and W. A. Lester, Jr., "Scattering Theory and Coupled-Channel Computations of Multiple-Surface Transitions in Nonreactive Collisions of F(²P) with H₂(¹ Σ_g^+)," Abstracts of the Xth International Conference on the Physics of Electronic and Atomic Collisions, Commissariat à l'Energie Atomique (Paris, France), p 766 (1977).
47. S. Green, B. J. Garrison, W. A. Lester, Jr., and W. H. Miller, "Collisional Excitation of Interstellar Formaldehyde," *Astrophys. J. (Supplement Series)* 37, 321 (1978).
48. A. W. Raczkowski, W. A. Lester, Jr., and W. H. Miller, "Vibrational Relaxation in the Para H₂-⁴He System: Comparison and Coupled-Channel, Coupled-States, and Effective Potential Methods," *J. Chem. Phys.* 69, 2692 (1978).
49. L. D. Thomas, W. A. Lester, Jr., and F. Rebentrost, "Classical Path Study of Nonadiabatic Transitions in Atom-Molecule Scattering: Quenching of F(²P_{1/2}) by H₂," *J. Chem. Phys.* 69, 5489 (1978).
50. R. E. Howard and W. A. Lester, Jr., "Ab Initio Calculation of Potential Energy Surfaces of the ¹A', ³A'', ¹A'', and ³B¹A' Potential Energy Surfaces of the O(³P, ¹D) + H₂(¹ Σ_g^+) Reaction," *Bull. Am. Phys. Soc.* 23, 1108 (1978).
51. R. Schinke and W. A. Lester, Jr., "Trajectory Studies of O + H₂ Reactions on Fitted ab initio Surfaces. I. Triplet Case," *J. Chem. Phys.* 70, 4893 (1979).
52. C. H. Becker, P. Casavecchia, Y. T. Lee, R. E. Olson, and W. A. Lester, Jr., "Coupled-Channel Study of Halogen (2P) + Rare Gas (1S) Scattering," *J. Chem. Phys.* 70, 5477 (1979).
53. A. C. Luntz, R. Schinke, W. A. Lester, Jr., and Hs. H. Gunthard, "Product State Distributions in the Reaction O(¹D₂) + H₂ → OH + H: Comparison of Experiment with Theory," *J. Chem. Phys.* 70, 5908 (1979).
54. R. E. Howard, A. D. McLean, and W. A. Lester, Jr., "Extended Basis First-Order CI Study of the ¹A', ³A'', and ³B¹A' Potential Energy Surfaces of the O(³P, ¹D) + H₂(¹ Σ_g^+) Reaction," *J. Chem. Phys.* 71, 2412 (1979).
55. R. Schinke and W. A. Lester, Jr., "Trajectory Studies of O + H₂ Reactions on Fitted ab initio Surfaces. II. Singlet Case," *J. Chem. Phys.* 72, 3754 (1980).
56. R. Schinke, M. Dupuis, and W. A. Lester, Jr., "Proton-H₂ Scattering on an ab initio Potential Energy Surface. I. Vibrational Excitation at 10 eV," *J. Chem. Phys.* 72, 3909 (1980).
57. W. A. Lester, Jr., "Recent Developments in Computational Chemistry in the US: The NRCC (National Resource for Computation in Chemistry)" in *Computational Methods in Chemistry*, Plenum (New York), p 301 (1980).
58. W. A. Lester, Jr., "De Vogelaere's Method" in *Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory*, ed. by L. D. Thomas, Vol. 1, p 105 (1980), Available as LBL-9501, UC-4, Conf.-790696 from the National Technical Information Services.
59. L. D. Thomas, M. H. Alexander, B. R. Johnson, W. A. Lester, Jr., J. C. Light, K. D. McLenithan, G. A. Parker, M. J. Redmon, T. G. Schmaltz, D. Secrest, and R. B. Walker, "Comparison of Numerical Methods for Solving the Second-Order Differential Equations of Molecular Scattering Theory," *J. Comput. Phys.* 41, 407 (1981).
60. V. Z. Kresin and W. A. Lester, Jr., "A New Adiabatic Approach to the Photodissociation of Polyatomic Molecules," *Int. J. Quantum Chem. Quantum Chem. Symp.* 15, 703 (1981).
61. Y. Osamura, H. F. Schaefer III, M. Dupuis, and W. A. Lester, Jr., "A Unimolecular Reaction ABC → A + B + C Involving Three Product Molecules and a Single Transition

- State. Photodissociation of Glyoxal: $\text{HCOHCO} \rightarrow \text{H}_2 + \text{CO} + \text{CO}$,” *J. Chem. Phys.* 75, 5828 (1981).
62. M. Dupuis, J. J. Wendoloski, T. Takada, and W. A. Lester, Jr., “Theoretical Study of Electrophilic Addition: $\text{O}(\text{^3P}) + \text{C}_2\text{H}_4$,” *J. Chem. Phys.* 76, 481 (1982).
63. M. Dupuis, J. J. Wendoloski, and W. A. Lester, Jr., “Electronic Structure of Vinoxy Radical CH_2CHO ,” *J. Chem. Phys.* 76, 488 (1982).
64. A. S. Dickinson, M. S. Lee, and W. A. Lester, Jr., “Close-Coupling Calculation of $\text{Li}^+ - \text{H}_2$ Diffusion Cross Sections,” *J. Phys. B* 15, 1371 (1982).
65. V. Z. Kresin and W. A. Lester, Jr., “Theory of Polyatomic Photodissociation. Adiabatic Description of the Dissociative State and the Translation-Vibration Interaction,” *J. Phys. Chem.* 86, 2182 (1982).
66. W. A. Lester, Jr., M. Dupuis, T. J. O'Donnell, and A. J. Olson, “Some Computational Trends in Theoretical Chemistry,” IUPAC Frontiers of Chemistry, Pergamon Press (New York), p 159 (1982).
67. V. Z. Kresin and W. A. Lester, Jr., “Inverse Vibrational Distributions of Photofragments,” *Chem. Phys. Lett.* 87, 392 (1982).
68. P. J. Reynolds, D. M. Ceperley, B. J. Alder, and W. A. Lester, Jr., “Fixed-Node Quantum Monte Carlo for Molecules,” *J. Chem. Phys.* 77, 5593 (1982).
69. W. A. Lester, Jr. and V. Z. Kresin, “A New Theoretical Method for Polyatomic Photodissociation,” *Bull. Am. Phys. Soc.* 28, 556 (1983).
70. W. A. Lester, Jr., book review, *Potential Energy Surfaces and Dynamics Calculations for Chemical Reactions and Molecular Energy Transfer*, D. G. Truhlar ed., *Am. Sci.*, 71, 214 (1983).
71. W. A. Lester, Jr., testimony on “Computers and Their Role in Energy Research: Current Status and Future Needs” in Hearings before the Subcommittee on Energy Development and Applications and the Subcommittee on Energy Research and Production of the Committee on Science and Technology, U.S. House of Representatives, Ninety-Eighth Congress, June 14 and 15, 1983, No. 20, U.S. Government Printing Office, Washington, DC, 1983.
72. M. Dupuis, W. A. Lester, Jr., B. H. Lengsfeld, III, and B. Liu, “Formaldehyde: *ab initio* MCSCF + CI Transition State for $\text{H}_2\text{CO} \rightarrow \text{CO} + \text{H}_2$ on the S_0 Surface,” *J. Chem. Phys.* 79, 6167 (1983).
73. M. Dupuis and W. A. Lester, Jr., “Hydrogen Atom Migration in the Oxidation of Aldehydes: $\text{O}(\text{^3P}) + \text{H}_2\text{CO}$,” *J. Chem. Phys.* 80, 4193 (1984).
74. M. Dupuis and W. A. Lester, Jr., “Hydrogen Atom Abstraction from Aldehydes: $\text{OH} + \text{H}_2\text{CO}$ and $\text{O} + \text{H}_2\text{CO}$,” *J. Chem. Phys.* 81, 847 (1984).
75. P. J. Reynolds and W. A. Lester, Jr., “Chemical Application of Diffusion Quantum Monte Carlo,” NASA Conference Pub. 2295, CYBER 200 Applications Seminar, 103 (1984).
76. R. M. Grimes, M. Dupuis, and W. A. Lester, Jr., “Static Dipole Polarizability of Electronically Excited Molecules: $\text{H}_2(\tilde{\text{B}}^1\Sigma_g^+)$,” *Chem. Phys. Lett.* 110, 247 (1984).
77. V. Z. Kresin and W. A. Lester, Jr., “Reaction Hamiltonian and the Adiabatic Approach to the Dynamics of Chemical Reaction,” *Chem. Phys.* 90, 335 (1984).
78. V. Z. Kresin, W. A. Lester, Jr., M. Dupuis, and C. E. Dateo, “Chemical Reaction as a Quantum Transition,” *Int. J. Quantum Chem. Quantum Chem. Symp.* 18, 691 (1984).
79. P. J. Reynolds, R. N. Barnett, and W. A. Lester, Jr., “Quantum Monte Carlo Study of the Classical Barrier Height for the $\text{H} + \text{H}_2$ Exchange Reaction: Restricted versus Unrestricted Trial Functions,” *Int. J. Quantum Chem. Quantum Chem. Symp.* 18, 709 (1984).
80. P. J. Reynolds, M. Dupuis, and W. A. Lester, Jr., “Quantum Monte Carlo Calculations of the Singlet-Triplet Splitting in Methylene,” *J. Chem. Phys.* 82, 1983 (1985).
81. R. N. Barnett, P. J. Reynolds, and W. A. Lester, Jr., “ $\text{H} + \text{H}_2$ Reaction Barrier: A Fixed-Node Quantum Monte Carlo Study,” *J. Chem. Phys.* 82, 2700 (1985).
82. C. E. Dateo, M. Dupuis, and W. A. Lester, Jr., “*Ab Initio* Study of Cyanogen: The $\tilde{\text{X}}^1\Sigma_g^+$, $\tilde{\alpha}^3\Sigma_u^+$, $\tilde{\text{B}}^1\Delta_u$, and $\tilde{\text{C}}^1\Pi_u$ States,” *J. Chem. Phys.* 83, 265 (1985).
83. V. Z. Kresin and W. A. Lester, Jr., “The Adiabatic Method in the Theory of Many-Body Systems” in *Mathematical Analysis of Physical Systems*, ed. R. E. Mickens, Van Nostrand Reinhold (New York), p 247 (1985).
84. W. A. Lester, Jr., V. Z. Kresin, and C. E. Dateo, “Adiabatic Approach in the Theory of Polyatomic Photodissociation: Application to C_2N_2 ,” in *Proceedings of the International Conference on Lasers '84*, eds., K. M. Corcoran, D. M. Sullivan, and W. C. Stwalley, STS Press (McLean, Virginia), p 499 (1985).
85. M. Dupuis and W. A. Lester, Jr., “Low-Lying Electronic States of Nitrosyl Cyanide (NCNO): An *ab initio* MCHF Study,” *J. Chem. Phys.* 83, 3990 (1985).
86. V. Z. Kresin and W. A. Lester, Jr., “Quantum Theory of Polyatomic Photodissociation,” *Adv. Photochem.* 13, 95 (1986).
87. M. Dupuis, G. Fitzgerald, B. Hammond, W. A. Lester, Jr., and H. F. Schaefer, III, “Theoretical Study of the $\text{H} + \text{O}_3 \leftrightarrow \text{OH} + \text{O}_2 \leftrightarrow \text{O} + \text{HO}_2$ System,” *J. Chem. Phys.* 84, 2691 (1986).
88. P. J. Reynolds and W. A. Lester, Jr., “Quantum Monte Carlo for Molecules,” *Phys. Today* 39, S-14 (1986).
89. R. N. Barnett, P. J. Reynolds, and W. A. Lester, Jr., “Electron Affinity of Flourine: A Quantum Monte Carlo Study,” *J. Chem. Phys.* 84, 4992 (1986).
90. P. J. Reynolds, R. N. Barnett, B. L. Hammond, R. M. Grimes, and W. A. Lester, Jr., “Quantum Chemistry by Quantum Monte Carlo: Beyond Ground-State Energy Calculations,” *Int. J. Quantum Chem.* 29, 589 (1986).
91. R. M. Grimes, W. A. Lester, Jr., and M. Dupuis, “Coupled-Channel Study of Rotational Excitation of an Electronically Excited Diatomic Molecule by Atom Impact: $\text{He}(\text{^1S}) + \text{H}_2(\text{B}^1\Sigma_g^+)$,” *J. Chem. Phys.* 84, 5437 (1986).
92. P. J. Reynolds, R. N. Barnett, B. L. Hammond, and W. A. Lester, Jr., “Molecular Physics and Chemistry Applications of Quantum Monte Carlo,” *J. Stat. Phys.* 43, 1017 (1986).
93. R. M. Grimes, B. L. Hammond, P. J. Reynolds, and W. A. Lester, Jr., “Quantum Monte Carlo Approach to Electronically Excited Molecules,” *J. Chem. Phys.* 84, 4749 (1986).
94. P. J. Reynolds, S. Alexander, D. Logan, and W. A. Lester, Jr., “Vector and Parallel Computers for Quantum Monte Carlo Computations” in Supercomputer Simulation in Chemistry, Lecture Notes in Chemistry, M. Dupuis, ed., Springer-Verlag (Berlin/New York), Vol. 44, p 280 (1986).
95. C. E. Dateo, V. Z. Kresin, M. Dupuis, and W. A. Lester, Jr., “Photodissociation as a Quantum Transition: Photofragment Vibrational Distributions of C_2N_2 ($\tilde{\text{C}}^1\Pi_u$) Predissociation,” *J. Chem. Phys.* 86, 2639 (1987).
96. M. Dupuis and W. A. Lester, Jr., “One-Electron Property from MCHF Wavefunction: The Dipole Moment of Ozone,” *Theor. Chim. Acta* 71, 255 (1987).

97. R. N. Barnett, P. J. Reynolds, and W. A. Lester, Jr., "Is Quantum Monte Carlo Competitive? Lithium Hydride Test Case," *J. Phys. Chem.* **91**, 2004 (1987).
98. B. L. Hammond, P. J. Reynolds, and W. A. Lester, Jr., "Valence Quantum Monte Carlo with *ab initio* Effective Core Potentials," *J. Chem. Phys.* **87**, 1130 (1987).
99. P. J. Reynolds, R. K. Owen, and W. A. Lester, Jr., "Is There a Zeroth Order Time-Step Error in Diffusion Quantum Monte Carlo?," *J. Chem. Phys.* **87**, 1905 (1987).
100. V. Z. Kresin and W. A. Lester, Jr., "On the Mechanism of Singlet-Triplet Transitions," *Chem. Phys. Lett.* **138**, 59 (1987).
101. M. N. Ramos, C. A. Taft, J. G. R. Tostes, and W. A. Lester, Jr., "An *ab initio* Spectroscopic Study of the HCN...HCN and HCN...HNC Linear Complexes," *J. Mol. Struct.* **175**, 303 (1988).
102. P. R. Seidl, K. Z. Leal, J. G. R. Tostes, C. A. Taft, B. L. Hammond, and W. A. Lester, Jr., "An *ab initio* Investigation of the Effects of 2-Exo and Endo Substituents on Norbornane," *Chem. Phys. Lett.* **147**, 373 (1988).
103. J. G. R. Tostes, C. A. Taft, M. N. Ramos, and W. A. Lester, Jr., "Role of Polarization Functions on the Bridge Hydrogen Atom in HCN...HCN," *Int. J. Quantum Chem.* **34**, 85 (1988).
104. C. A. Taft, J. C. Azevedo, J. G. R. Tostes, and W. A. Lester, Jr., "Ab Initio Studies of the Linear HC₃N...HC₃N Complex," *J. Mol. Struct. (THEOCHEM)* **168**, 169 (1988).
105. B. L. Hammond, P. J. Reynolds, and W. A. Lester, Jr., "Damped-Core Quantum Monte Carlo Method: Effective Treatment for Large-Z Systems," *Phys. Rev. Lett.* **61**, 2312 (1988).
106. M. Braga, A. L. Almeida, C. A. Taft, B. L. Hammond, and W. A. Lester, Jr., "Theoretical Study of the Interaction of Fe, Fe+, and FeCO with Ar," *J. Chem. Phys.* **89**, 4867 (1988).
107. M. Braga, S. K. Lie, C. A. Taft, and W. A. Lester, Jr., "Electronic Structure, Hyperfine Interactions, and Magnetic Properties for Iron Octahedral Sulfides," *Phys. Rev. B* **38**, 10837 (1988).
108. Z. Sun, P. J. Reynolds, R. K. Owen, and W. A. Lester, Jr., "Monte Carlo Study of Electron Correlation Functions for Small Molecules," *Theo. Chim. Acta* **75**, 353 (1989).
109. V. Z. Kresin and W. A. Lester, Jr., "Reaction Hamiltonian Method for Chemical Reactions: Effect of Indistinguishable Nuclei," *Chem. Phys. Lett.* **159**, 297 (1989).
110. A. C. Pavao, C. A. Taft, B. L. Hammond, and W. A. Lester, Jr., "Molecular Cluster Model for Magnetic Iron," *Phys. Rev. B* **40**, 2879 (1989).
111. P. Pernot, R. M. Grimes, W. A. Lester, Jr., and Ch. Cerjan, "Quantum Time-Dependent Study of the Scattering of He by H₂(B ¹S_u⁺)," *Chem. Phys. Lett.* **163**, 297 (1989).
112. V. Z. Kresin and W. A. Lester, Jr., "Nonadiabatic Hamiltonian for Electronic-Vibrational Coupling," *Int. J. Quantum Chem. Quantum Chem. Symp.* **23**, 17 (1989).
113. S.-Y. Huang, Z. Sun, and W. A. Lester, Jr., "Optimized Trial Functions for Quantum Monte Carlo," *J. Chem. Phys.* **92**, 597 (1990).
114. P. R. Seidl, K. Z. Leal, J. W. M. Carneiro, J. G. R. Tostes, C. A. Taft, B. L. Hammond, and W. A. Lester, Jr., "Ab Initio Charge Distributions in Half-Cage Compounds," *J. Mol. Struct. (THEOCHEM)* **204**, 183 (1990).
115. B. Kim, B. L. Hammond, W. A. Lester, Jr., and H. S. Johnston, "Ab Initio Study of Vibrational Spectra of NO₃," *Chem. Phys. Lett.* **168**, 131 (1990).
116. B. Bernu, D. M. Ceperley, and W. A. Lester, Jr., "The Calculation of Excited States with Quantum Monte Carlo. II. Vibrational Excited States," *J. Chem. Phys.* **93**, 552 (1990).
117. B. L. Hammond, W. A. Lester, Jr., M. Braga, and C. A. Taft, "Theoretical Study of the Interaction of Ionized Transition Metals (Cr, Mn, Fe, Co, Ni, Cu) with Argon," *Phys. Rev. B* **41**, 10447 (1990).
118. Z. Z. Yang, L. S. Wang, Y. T. Lee, D. A. Shirley, S.-Y. Huang, and W. A. Lester, Jr., "Molecular Beam Photoelectron Spectroscopy of Allene," *Chem. Phys. Lett.* **171**, 9 (1990).
119. Z. Sun, S.-Y. Huang, R. N. Barnett, and W. A. Lester, Jr., "Wavefunction Optimization with a Fixed Sample in Quantum Monte Carlo," *J. Chem. Phys.* **93**, 3326 (1990).
120. B. L. Hammond, S.-Y. Huang, W. A. Lester, Jr., and M. Dupuis, "Theoretical Study of the O(³P) + Allene Reaction," *J. Phys. Chem.* **94**, 7969 (1990).
121. W. A. Lester, Jr. and B. L. Hammond, "Quantum Monte Carlo for the Electronic Structure of Atoms and Molecules," *Annu. Rev. Phys. Chem.* **41**, 283 (1990).
122. W. A. Lester, Jr., "Supercomputing and Research in Theoretical Chemistry," in *Energy Sciences Supercomputing 1990*, National Energy Research Supercomputer Center, Lawrence Livermore National Laboratory (Livermore, California), 1990.
123. A. C. Pavao, M. Braga, C. A. Taft, B. L. Hammond, and W. A. Lester, Jr., "Theoretical Study of the CO Interaction with 3d Metal Surface," *Phys. Rev. B* **43**, 6962 (1991).
124. P. Pernot and W. A. Lester, Jr., "Quantum Time-Dependent Treatment of Molecular Collisions: Scattering of He by H₂(B ¹S_u⁺)," *Comput. Phys. Commun.* **63**, 259 (1991).
125. A. C. Pavao, M. Braga, C. A. Taft, B. L. Hammond, and W. A. Lester, Jr., "Theoretical Study of the CO Interaction with the Fe(100) Surface," *Phys. Rev. B* **44**, 1910 (1991).
126. P. Pernot and W. A. Lester, Jr., "Multidimensional Wave-Packet Analysis: Splitting Method for Time-Resolved Property Determination," *Int. J. Quantum Chem.* **40**, 577 (1991).
127. B. L. Hammond, M. M. Soto, R. N. Barnett, and W. A. Lester, Jr., "On Quantum Monte Carlo for the Electronic Structure of Molecules," *J. Mol. Struct. (THEOCHEM)* **234**, 525 (1991).
128. R. N. Barnett, P. J. Reynolds, and W. A. Lester, Jr., "Monte Carlo Algorithms for Expectation Values of Coordinate Operators," *J. Comput. Phys.* **96**, 258 (1991).
129. R. N. Barnett, P. J. Reynolds, and W. A. Lester, Jr., "Computation of Transition Dipole Moments by Monte Carlo," *J. Chem. Phys.* **96**, 2141 (1992).
130. Z. Sun, R. N. Barnett, and W. A. Lester, Jr., "Optimization of a Multideterminant Wave Function for Quantum Monte Carlo," *J. Chem. Phys.* **96**, 2422 (1992).
131. J. S. Francisco, Y. Zhao, W. A. Lester, Jr., and I. H. Williams, "Theoretical Studies of the Structure and Thermochemistry of FO₂ Radical: Comparison of Moller-Plesset Perturbation, Complete-Active-Space Self-Consistent-Field, and Quadratic Configuration Interaction Methods," *J. Chem. Phys.* **96**, 2861 (1992).
132. R. N. Barnett, P. J. Reynolds, and W. A. Lester, Jr., "Monte Carlo Determination of the Oscillator Strength and Excited State Lifetime for the Li 2²S → 2²P Transition," *Int. J. Quantum Chem.* **42**, 837 (1992).
133. Z. Sun, R. N. Barnett, and W. A. Lester, Jr., "Quantum and Variational Monte Carlo Interaction Potentials for Li₂(X ¹S_g⁺)," *Chem. Phys. Lett.* **195**, 365 (1992).
134. V. Z. Kresin and W. A. Lester, Jr., "A Quantum Mechanical Model of Heterogeneous Catalysis," *Chem. Phys. Lett.* **197**, 1 (1992).

135. Z. Sun, W. A. Lester, Jr., and B. L. Hammond, "Correlated Sampling of Monte Carlo Derivatives with Iterative-Fixed Sampling," *J. Chem. Phys.* **97**, 7585 (1992).
136. W. A. Glauser, W. R. Brown, W. A. Lester, Jr., D. Bressanini, B. L. Hammond, and M. L. Kosykowski, "Random-Walk Approach to Mapping Nodal Regions of N-Body Wave Functions: Ground-State Hartree-Fock Wave Functions for Li-C," *J. Chem. Phys.* **97**, 9200 (1992).
137. J. W. de M. Carneiro, P. R. Seidl, J. G. R. Tostes, C. A. Taft, B. L. Hammond, M. M. Soto, and W. A. Lester, Jr., "The Effects of Lone Pairs on Charge Distribution in the Tetracyclic Norbornyl Derivatives," *Chem. Phys. Lett.* **202**, 278 (1993).
138. J. A. Odutola, W. A. Lester, Jr., and R. M. Grimes, "Reorientation Cross Sections in Collisions of He(¹S) + H₂(B ¹ Σ_u^+)," *J. Chem. Phys.* **99**, 2632 (1993).
139. Z. Sun, M. M. Soto, and W. A. Lester, Jr., "Characteristics of Electron Movement in Variational Monte Carlo Simulations," *J. Chem. Phys.* **100**, 1278 (1994).
140. J. G. R. Tostes, J. W. de M. Carneiro, S. K. Lie, P. R. Seidl, C. A. Taft, M. M. Soto, W. A. Lester, Jr., and B. L. Hammond, "Hyperconjugation and Charge Distribution in Alicyclic Alcohols and Exo- and Endo-Norbornol," *J. Mol. Struct. (THEOCHEM)* **306**, 101 (1994).
141. B. L. Hammond, W. A. Lester, Jr., and P. J. Reynolds, *Monte Carlo Methods in Ab Initio Quantum Chemistry*, World Scientific (Singapore) (1994).
142. Z. Sun, M. M. Soto, R. N. Barnett, and W. A. Lester, Jr., "An Approach for Improved Variational Quantum Monte Carlo," *J. Chem. Phys.* **101**, 394 (1994).
143. A. C. Pavão, M. M. Soto, W. A. Lester, Jr., S. K. Lie, B. L. Hammond, and C. A. Taft, "Molecular States of CO Interaction with 3d-Metal Surfaces," *Phys. Rev. B* **50**, 1868 (1994).
144. J. A. Odutola and W. A. Lester, Jr., "Molecular Reorientation in Cross Sections in Collisions of He (¹S) + H₂(B ¹ Σ_u^+), HD(B ¹ Σ_u^+)," *J. Chem. Phys.* **101**, 9619 (1994).
145. A. C. Pavão, B. L. Hammond, M. M. Soto, W. A. Lester, Jr., and C. A. Taft, "Theoretical Study of the CO Interaction with the Cr (110) Surface," *Surf. Sci.* **323**, 340 (1995).
146. R. N. Barnett, E. M. Johnson, and W. A. Lester, Jr., "Quantum Monte Carlo Determination of the Lithium 2²S → 2²P Oscillator Strength: Higher Precision," *Phys. Rev. A* **51**, 2049 (1995).
147. J. Glauco, R. Tostes, P. R. Seidl, M. M. Soto, J. W. de M. Carneiro, S. K. Lie, C. A. Taft, W. Brown, and W. A. Lester, Jr., "Ab Initio Studies of Hyperconjugation Effects on Charge Distribution in Tetracyclododecane Alcohols," *Chem. Phys. Lett.* **237**, 33 (1995).
148. W. A. Lester, Jr., "Quantum Monte Carlo for Molecules: Method and Applications" in Proceedings, Sixth Annual Conference of the National Alliance of Research Centers of Excellence, p. 6 (1994). Available from The Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia.
149. A. C. Pavão, C. A. Taft, T. C. Guimaraes, and W. A. Lester, Jr., "Breaking Bonds of Diatomic Molecules on Transition Metal Surfaces," *Recent Trends Chem. Phys.* **3**, 109 (1994).
150. W. R. Brown, W. A. Glauser, and W. A. Lester, Jr., "Quantum Monte Carlo for Floppy Molecules. Vibrational States of C₃," *J. Chem. Phys.* **103**, 9721 (1995).
151. C. A. Taft, P. R. Seidl, J. G. R. Tostes, S. K. Lie, J. W. de M. Carneiro, and W. A. Lester, Jr., "Ab Initio Study of Hyperconjugation Effects on Charge Distribution in Representative Polycyclic Alcohols," *Chem. Phys. Lett.* **248**, 158 (1996).
152. C. W. Greeff, W. A. Lester, Jr., and B. L. Hammond, "Electronic States of Al and Al₂ using Quantum Monte Carlo with an Effective Core Potential," *J. Chem. Phys.* **104**, 1973 (1996).
153. J. G. R. Tostes, P. R. Seidl, C. A. Taft, S. K. Lie, J. W. De M. Carneiro, W. Brown, and W. A. Lester, Jr., "Carbon-Carbon and Carbon-Hydrogen Hyperconjugation in Neutral Alcohols," *J. Mol. Struct. (THEOCHEM)* **388**, 85 (1996).
154. C. W. Greeff and W. A. Lester, Jr., "Quantum Monte Carlo Binding Energies for Silicon Hydrides," *J. Chem. Phys.* **106**, 6412 (1997).
155. R. N. Barnett and W. A. Lester, Jr., "Quantum Monte Carlo and Electronic Structure," *Computational Chemistry: Review of Current Trends*, ed. J. Leszczynski, World Scientific Publishing (Singapore), p 125 (1997).
156. W. A. Lester, Jr., Editor, *Recent Advances in Quantum Monte Carlo Methods*, World Scientific (Singapore), (1997).
157. C. W. Greeff, W. A. Lester, Jr., and B. L. Hammond, "Quantum Monte Carlo with Pseudopotentials for Electronic Structure of Atoms and Molecules" in *Recent Advances in Quantum Monte Carlo Methods*, ed. W. A. Lester, Jr., World Scientific Publishing (Singapore), p 117 (1997).
158. R. N. Barnett, Z. Sun, and W. A. Lester, Jr., "Fixed-Sample Optimization in Quantum Monte Carlo Using a Probability Density Function," *Chem. Phys. Lett.* **273**, 321 (1997).
159. T. C. Guimaraes, A. C. Pavão, C. A. Taft, and W. A. Lester, Jr., "Interaction Mechanism of N₂ with the Cr (110) Surface," *Phys. Rev. B* **56**, 7001 (1997).
160. C. W. Greeff and W. A. Lester, Jr., "A Soft Hartree-Fock Pseudopotential for Carbon with Application to Quantum Monte Carlo," *J. Chem. Phys.* **109**, 1607 (1998).
161. W. A. Lester, Jr. and R. N. Barnett, "Quantum Monte Carlo Methods for Electronic Structure," in *The Encyclopedia of Computational Chemistry*, eds. P. v. R. Schleyer, N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, H. F. Schaefer, III, P. R. Schreiner, John Wiley & Sons (Chichester, U.K.), Vol. 3, p 1735 (1998).
162. A. L. Almeida, J. B. L. Martins, C. A. Taft, E. Longo, and W. A. Lester, Jr., "Ab Initio and Semiempirical Studies of the Adsorption and Dissociation of Water on Pure, Defective, and Doped MgO (001) Surfaces," *J. Chem. Phys.* **109**, 3671 (1998).
163. A. C. Pavao, T. C. F. Guimaraes, S. K. Lie, C. A. Taft, and W. A. Lester, Jr., "Modeling the Adsorption and Dissociation of CO on Transition Metal Surfaces," *J. Mol. Struct. (THEOCHEM)* **458**, 99 (1999).
164. A. L. Almeida, J. B. L. Martins, C. A. Taft, E. Longo, and W. A. Lester, Jr., "Theoretical Study of Water Coverage on MgO Surfaces," *Int. J. Quantum Chem.* **71**, 153 (1999).
165. J. C. Grossman, W. A. Lester, Jr., and S. G. Louie, "Cyclopentadiene Stability: Quantum Monte Carlo, Coupled Cluster, and Density Functional Theory Determinations," *Mol. Phys.* **96**, 629 (1999).
166. C. A. Taft, T. C. Guimaraes, A. C. Pavão, and W. A. Lester, Jr., "Adsorption and Dissociation of Diatomic Molecules on Transition Metal Surfaces," *Int. Rev. Phys. Chem.* **18**, 163 (1999).
167. T. C. Guimaraes, A. C. Pavão, C. A. Taft, and W. A. Lester, Jr., "Dissociation of N₂ on Chromium Alloys: A General Mechanism for Dissociation of Diatomic Molecules," *Phys. Rev. B* **60**, 11789 (1999).
168. X. Krokidis, N. W. Moriarty, W. A. Lester, Jr., and M. Frenklich, "Propargyl Radical: An Electron Localization Function Study," *Chem. Phys. Lett.* **314**, 541 (1999).

169. J. C. Grossman, W. A. Lester, Jr., and S. G. Louie, "Quantum Monte Carlo and Density Functional Theory Characterization of 2-Cyclopentenone and 3-Cyclopentenone Formation from O(³P) + Cyclopentadiene, *J. Am. Chem. Soc.* 122, 705 (2000).
170. J. A. W. Harkless and W. A. Lester, Jr., "Quantum Monte Carlo for Atoms and Molecules," Proceedings of the Workshop on Contemporary Problems in Mathematical Physics, World Scientific Publishing (Singapore), p 153 (2000).
171. J. A. W. Harkless and W. A. Lester, Jr., "Quantum Monte Carlo Determination of the Atomization Energy and Heat of Formation of Propargyl Radical," *J. Chem. Phys.* 113, 2680 (2000).
172. R. N. Barnett, Z. Sun, and W. A. Lester, Jr., "Improved Trial Wave Functions in Quantum Monte Carlo: Application to Acetylene and Its Dissociation Fragments," *J. Chem. Phys.* 114, 2013 (2001).
173. A. C. Pavão, C. A. Taft, T. C. F. Guimaraes, M. B. C. Leão, J. R. Mohallem, and W. A. Lester, Jr. "Interdisciplinary Applications of Pauling's Metallic Orbital and Unsynchroized Resonance to Problems of Modern Physical Chemistry: Conductivity, Magnetism, Molecular Stability, Superconductivity, Catalysis, Photoconductivity and Chemical Reaction," (Feature Article), *J. Phys. Chem. A* 105, 5 (2001).
174. C. A. Taft, E. Longo, F. Sensato, J. B. L. Martins, R. Sambrano, A. L. Almeida, and W. A. Lester, Jr. "Interaction of Water, Gases and Other Complexes with Metal Oxide Surfaces," *Recent Res. Devel. Quantum Chem.* 1, 105 (2000).
175. I. V. Ovcharenko, A. Aspuru-Guzik, and W. A. Lester, Jr., "Soft Pseudopotentials for Efficient Quantum Monte Carlo Calculations: From Be to Ne and Al to Ar," *J. Chem. Phys.* 114, 7790 (2001).
176. I. V. Ovcharenko, W. A. Lester, Jr., C. Xiao, and F. Hagelberg, "Quantum Monte Carlo Characterization of Small Cu-Doped Silicon Clusters: CuSi₄ and CuSi₆," *J. Chem. Phys.* 114, 9028 (2001).
177. C. Xiao, F. Hagelberg, I. Ovcharenko, and W. A. Lester, Jr., "Geometric Structures and Stabilities of CuSi_n Clusters (n=8, 10, 12)," *J. Mol. Struct. (THEOCHEM)* 549, 181 (2001).
178. W. A. Lester, Jr., "Research Developments and Progress During the Nineties," *J. Mol. Struct. (THEOCHEM)* 573, 55 (2001).
179. X. Krokidis, N. W. Moriarty, W. A. Lester, Jr., and M. Frenklach, "A Quantum Monte Carlo Study of Energy Differences in C₄H₃ and C₄H₅ Isomers," *Int. J. Chem. Kinet.* 33, 808 (2001).
180. A. L. Almeida, J. B. L. Martins, E. Longo, N. C. Furtado, C. A. Taft, J. R. Sambrano, and W. A. Lester, Jr., "Theoretical study of MgO(001) surfaces: pure, doped with Fe, Ca, and Al, and with and without adsorbed water," *Int. J. Quantum Chem.* 84, 705 (2001).
181. C. Xiao, F. Hagelberg, and W. A. Lester, Jr., "Geometric, Energetic and Bonding Properties of Neutral and Charged Copper-Doped Silicon Clusters," *Phys. Rev. B* 66 075425-1 (2002).
182. W. A. Lester, Jr. and J. C. Grossman, "Quantum Monte Carlo for the Electronic Structure of Combustion Systems," in *Recent Advances in Quantum Monte Carlo – Part II*, eds., W. A. Lester, Jr., S. Rothstein, and S. Tanaka, World Scientific Publishing (Singapore), p 159 (2002).
183. C. Xiao, A. Abraham, R. Quinn, F. Hagelberg, and W. A. Lester, Jr., "Comparative study on the interaction of Scandium and Copper atoms with small silicon clusters," *J. Phys. Chem. A* 106, 11380 (2002).
184. F. Hagelberg, C. Xiao, and W. A. Lester, Jr., "Cage-like Si₁₂ Clusters with Endohedral Cu, Mo and W Metal Atom Impurities," *Phys. Rev. B* 67, 35426 (2003).
185. O. El Akramine, W. A. Lester, Jr., X. Krokidis, C. A. Taft, T. C. Guimaraes, A. C. Pavao, and R. Zhu, "Quantum Monte Carlo Study of the CO Interaction with a Model Surface for Cr(110)," *Mol. Phys.* 101, 277 (2003).
186. J. A. W. Harkless, J. H. Rodriguez, L. Mitas, and W. A. Lester, Jr., "A Quantum Monte Carlo and Density Functional Theory Study of Peroxynitrite Anion," *J. Chem. Phys.* 118, 4987 (2003).
187. O. El Akramine, A. C. Kollias, and W. A. Lester, Jr., "Quantum Monte Carlo Study of the Singlet-Triplet Transition in Ethylene," *J. Chem. Phys.* 119, 1483 (2003).
188. A. C. Kollias and W. A. Lester, Jr., "Quantum Monte Carlo and Electron Localization Function Study of the Electronic Structure of CO₂₊," *J. Mol. Struct. (THEOCHEM)* 634, 1 (2003).
189. A. Aspuru-Guzik and W. A. Lester, Jr., "Quantum Monte Carlo for the Solution of the Schroedinger Equation for Molecular Systems," in *Special Volume Computational Chemistry*, ed. C. Le Bris, *Handbook of Numerical Analysis*, ed. P. G. Ciarlet, Elsevier (Amsterdam), p 485 (2003).
190. C. Schuetz, M. Frenklach, A. C. Kollias, and W. A. Lester Jr., "Geometry Optimization in Quantum Monte Carlo with Solution Mapping: Application to Formaldehyde," *J. Chem. Phys.* 119, 9386 (2003).
191. A. Aspuru-Guzik, M. H. Kalos, and W. A. Lester, Jr., "Fermion Monte Carlo Study of the Beryllium Atom," *The Monte Carlo Method in the Physical Sciences*, ed. J. E. Gubernatis, American Institute of Physics (Melville, NY), p 371 (2003).
192. A. Aspuru-Guzik, O. El Akramine, J. C. Grossman, and W. A. Lester, Jr., "Quantum Monte Carlo for Electronic Excitations of Free-Base Porphyrin," *J. Chem. Phys.* 120, 3049 (2004).
193. G. Hill, G. Forde, N. Hill, W. A. Lester, Jr., W. A. Sokalski, and J. Leszczynski, "Interaction Energies in Stacked DNA Bases? How Important are Electrostatics?" *Chem. Phys. Lett.* 381, 729 (2003).
194. A. C. Kollias, O. Couronne, and W. A. Lester, Jr., "Quantum Monte Carlo Study of the Reaction: Cl + CH₃OH → CH₂OH + HCl," *J. Chem. Phys.* 121, 1357 (2004).
195. A. Aspuru-Guzik and W. A. Lester, Jr., "Quantum Monte Carlo: Theory and Application to Molecular Systems," *Proceedings of the International Conference on Computational and Mathematical Methods in Science and Engineering*, CMMSE-2004, Uppsala, June 4-8, 2004, p 100.
196. A. Aspuru-Guzik and W. A. Lester, Jr., "Studying Biological Molecules with Quantum Monte Carlo: Improved scaling", Abstract, 228th ACS National Meeting, Philadelphia, PA, August 2004.
197. W. A. Lester, Jr., Commentary on "Quantum Monte Carlo Studies on Be and LiH," in *Molecular Quantum Mechanics, Selected papers of N. C. Handy*, eds. D. C. Clary, S. M. Colwell, and H. F. Schaefer III, p 145 (2004).
198. A. Aspuru-Guzik, R. Salomon-Ferrer, B. Austin, and W. A. Lester, Jr., "A Sparse Algorithm for the Evaluation of the Local Energy in Quantum Monte Carlo," *J. Comput. Chem.* 26, 708 (2005).
199. A. Aspuru-Guzik, R. Salomon-Ferrer, B. Austin, R. Perusquia-Flores, M. A. Griffin, R. A. Oliva, D. Skinner, D.

- Domin, and W. A. Lester, Jr., "Zori 1.0: A Parallel Quantum Monte Carlo Electronic Package," *J. Comput. Chem.* 26, 856 (2005).
200. A. Aspuru-Guzik, A. C. Kollas, R. Salomon-Ferrer, and W. A. Lester, Jr. "Quantum Monte Carlo: Theory and Applications to Atomic, Molecular and Nano Systems," in *Handbook of Theoretical and Computational Nanotechnology*, eds. M. Rieth and W. Schommers, American Scientific Publishers (Stevenson Ranch, CA) (2005).
201. A. C. Kollas, D. Domin, G. Hill, M. Frenklach, D. M. Golden, and W. A. Lester, Jr., "Quantum Monte Carlo Study of Heats of Formation and Bond Dissociation Energies of Small Hydrocarbons," *Int. J. Chem. Kinet.* 37, 583 (2005).
202. W. A. Lester, Jr., FOREWORD to Beyond Small Numbers: Voices of African American PhD Chemists by Willie Pearson, Jr., Volume 4 of the series, Diversity in Higher Education, Elsevier (Amsterdam), p xvii (2005).
203. A. C. Kollas, D. Domin, G. Hill, M. Frenklach, and W. A. Lester, Jr., "Quantum Monte Carlo Study of Small Hydrocarbon Atomization Energies," *Mol. Phys.* 104, 467 (2006). Article written in honor of Nicholas Handy.
204. A. Aspuru-Guzik and W. A. Lester, Jr., "Quantum Monte Carlo: Theory and Application to Molecular Systems," *Adv. Quantum Chem.* 49, 209 (2005).
205. R. Whitesides, A. C. Kollas, D. Domin, W. A. Lester, Jr., and M. Frenklach, "Graphene Layer Growth: Collision of Migrating 5-Member Rings," Fall Meeting of the Western States Section of the Combustion Institute, Stanford, CA, October 17–18, 2005, paper 05F-62.
206. W. A. Lester, Jr. and R. Salomon-Ferrer, "Some Developments in Quantum Monte Carlo for Electronic Structure: Methods and Application to a Bio System," *THEOCHEM* 771, 51 (2006).
207. P. T. A. Galek, N. C. Handy, and W. A. Lester, Jr. "Quantum Monte Carlo Studies on Small Molecules," *Mol. Phys.* 104, 3069 (2006).
208. R. Whitesides, A. C. Kollas, D. Domin, W. A. Lester, Jr., and M. Frenklach, "Graphene Layer Growth: Collision of Migrating Five-Member Rings," *Proc. Combust. Inst.* 31, 539 (2007).
209. B. Austin, A. Aspuru-Guzik, R. Salomon-Ferrer, and W. A. Lester, Jr., "Linear – Scaling Evaluation of the Local Energy in Quantum Monte Carlo," in *Proceedings of the Pacificchem Symposium on Advances in Quantum Monte Carlo*, eds. J. B. Anderson and S. M. Rothstein, ACS Symposium Series, American Chemical Society (Washington, DC), No. 953, p 55 (2007).
210. R. Prasad, N. Umezawa, D. Domin, R. Salomon-Ferrer, and W. A. Lester, Jr., "Quantum Monte Carlo Study of First-Row Atoms using Transcorrelated Variational Monte Carlo Trial Functions," *J. Chem. Phys.* 126, 164109 (2007).
211. C. Amador-Bedolla, R. Salomon-Ferrer, J. A. Vazquez-Martinez, and W. A. Lester, Jr., "Reagents for Electrophilic Amination: A Quantum Monte Carlo Study," *J. Chem. Phys.* 126, 204308 (2007).
212. R. Whitesides, D. Domin, R. Salomon-Ferrer, W. A. Lester, Jr., and M. Frenklach, "Graphene Layer Growth Chemistry: Five- and Six-Member Ring Flip Reaction," *J. Phys. Chem. A* 112, 2125 (2008).
213. M. T. Nguyen, M. H. Matus, W. A. Lester, Jr., and D. A. Dixon, "Heats of Formation of Triplet Ethylene, Ethylidene, and Acetylene," *J. Phys. Chem. A* 112, 2082 (2008).
214. D. Domin, W. A. Lester, Jr., R. Whitesides, and M. Frenklach, "Isomer Energy Differences for the C₄H₃ and C₄H₅ Isomers Using Diffusion Monte Carlo," *J. Phys. Chem. A* 112, 2065 (2008).