

# Publications

1. D.L. Freeman, "The Interaction of Rare Gas Atoms with Graphite Surfaces. I. Single Adatom Energies," J. Chem. Phys., **62**, 941-949 (1975).
2. D.L. Freeman, "The Interaction of Rare Gas Atoms with Graphite Surfaces. II. Adatom-Adatom Potentials," J. Chem. Phys., **62**, 4300-4307 (1975).
3. D.L. Freeman and M. Karplus, "Many-body Perturbation Theory Applied to Molecules: Analysis and Correlation Energy Calculation for  $\text{Li}_2$ ,  $\text{N}_2$ , and  $\text{H}_3$ ," J. Chem. Phys., **64**, 2641- 2659 (1976).
4. D.L. Freeman, "The Coupled-cluster Expansion Applied to the Electron Gas: Inclusion of Ring and Exchange Effects," Phys. Rev. B**15**, 5512-5521 (1977).
5. D.L. Freeman, "Application of the Coupled-cluster Expansion to the Correlation Energy of Electrons in Two-dimensional and Quasi-two-dimensional Systems," Solid State Commun., **26**, 289-293 (1978).
6. N.C. Dutta and D.L. Freeman, "A Numerical Solution to the Integral Equation for Atomic Pair Energies," Mol. Phys. **36**, 655- 667 (1978).
7. J.D. Pack, H.J. Monkhorst, and D.L. Freeman, "Lithium Crystal Properties from High-quality Hartree-Fock Wave Functions," Solid State Commun., **29**, 723-725 (1979).
8. J.D. Pack, H.J. Monkhorst, and D.L. Freeman, "On the X-ray Scattering Factors of Metallic and Molecular Hydrogen Crystals," Solid State Commun., **29**, 735-737 (1979).
9. D.L. Freeman, "Coupled-cluster Summation of the Particle-Particle Ladder Diagrams for the Two-dimensional Electron Gas," J. Phys. C.: Solid State Physics, **16**, 711-727 (1983).
10. D.L. Freeman and J.D. Doll, "The Influence of Diffusion on Surface Reaction Kinetics," J. Chem. Phys., **78**, 6002-6009 (1983).
11. D.L. Freeman and J.D. Doll, "Langevin Analysis of the Diffusion Model for Surface Chemical Reactions," J. Chem. Phys., **79**, 2343-2350 (1983).

12. J.D. Doll and D.L. Freeman, "A Monte-Carlo/Molecular Dynamics Study of the Diffusional Recombination Kinetics of  $C_{(a)}+O_{(a)} \rightarrow CO_{(g)}$  on Pt(III)," *Surf. Sci.*, **134**, 769-776 (1983).
13. J.D. Doll and D.L. Freeman, "A Monte-Carlo Method for Quantum-Boltzmann Statistical Mechanics," *J.Chem. Phys.*, **80**, 2239-2240 (1984).
14. D.L. Freeman and J.D. Doll, "A Monte Carlo-Method for Quantum-Boltzmann Statistical Mechanics Using Fourier Representations of Path Integrals," *J. Chem. Phys.*, **80**, 5709-5718 (1984).
15. D.L. Freeman and J.D. Doll, "Quantum Monte-Carlo Study of the Thermodynamic Properties of Argon Clusters: The Homogeneous Nucleation of Argon in Argon Vapor and 'Magic Number' Distributions in Argon Vapor," *J. Chem. Phys.*, **82**, 462-471 (1985).
16. J.D. Doll, R.D. Coalson, and D.L. Freeman, "Fourier Path-Integral Monte-Carlo Methods: Partial Averaging," *Phys. Rev. Lett.*, **55**, 1-4 (1985).
17. J.D. Doll and D.L. Freeman, "A Comparison of Energy Estimators Used in Quantum Monte-Carlo Calculations," *J. Chem. Phys.*, **83**, 768-771 (1985).
18. D.L. Freeman, R.D. Coalson and J.D. Doll, "Fourier Path Integral Methods: A Model Study of Simple Fluids," *J. Stat. Phys.*, **43**, 931-934 (1986).
19. R.D. Coalson, D.L. Freeman and J.D. Doll, "Partial Averaging Approach to Fourier Coefficient Path Integration," *J. Chem. Phys.*, **85**, 4567-4583 (1986).
20. J.D. Doll and D.L. Freeman, "Randomly Exact Methods," *Science*, **234**, 1356-1360 (1986).
21. J. D. Doll and D.L. Freeman, "A Time for Noise: Random Methods and Chemical Theory," *Chem. Design Auto. News*, **2**, 1-4 (1987).
22. J.D. Doll, R.D. Coalson and D.L. Freeman, "Toward a Monte Carlo Theory of Quantum Dynamics," *J. Chem. Phys.*, **87**, 1641-1647 (1987).
23. D.L. Freeman and J.D. Doll, "The Quantum Mechanics of Clusters," *Adv. Chem. Phys.*, **70**, 139 (1988).
24. J.D. Doll and D.L. Freeman, "Stationary Phase Monte Carlo Methods," *Adv. Chem. Phys.*, **73**, 289 (1989).
25. J.D. Doll and D.L. Freeman, "A Comparative Analysis of Stationary Phase Monte Carlo Methods," *J. Phys. Chem.*, **92**, 3278 (1988).

26. J.D. Doll, D.L. Freeman and M.J. Gillan, "Stationary Phase Monte Carlo Methods: An Exact Formulation," *Chem. Phys. Lett.*, **143**, 277 (1988).
27. J.D. Doll, T.L. Beck and D.L. Freeman, "A Quantum Monte Carlo Dynamics: The Stationary Phase Monte Carlo Path Integral Calculation of Finite Temperature Time Correlation Functions," *J. Chem. Phys.*, **89**, 5753 (1988).
28. J.A. Northby, J. Xie, D.L. Freeman and J.D. Doll, "Binding Energy of Large Icosahedral and Cuboctahedral Lennard-Jones Clusters," *Z. Phys. D-Atoms, Molecules and Clusters*, **12**, 69 (1989)
29. J.D. Doll, D.L. Freeman and A. Voter, "Recent Developments in the Theory of Many-body Processes: Implications for the Study of Surface Dynamics," in *Diffusion at Interfaces: Microscopic Concepts*, M. Grunze, H.J. Kreuzer and J.J. Weimer, Eds., Springer Series in Surface Sciences, **12**, 144 (Springer, Berlin, 1988).
30. T.L. Beck, J.D. Doll and D.L. Freeman, "Locating Stationary Paths in Functional Integrals: An Optimization Method Utilizing the Stationary Phase Monte Carlo Sampling Function," *J. Chem. Phys.* **90**, 3181 (1989).
31. T.L. Beck, J.D. Doll and D.L. Freeman, "The Quantum Mechanics of Cluster Melting," *J. Chem. Phys.*, **90**, 5651 (1989).
32. J. Xie, J.A. Northby, D.L. Freeman and J.D. Doll, "Theoretical Studies of the Energetics and Structure of Atomic Clusters," *J. Chem. Phys.*, **91**, 612 (1989).
33. K.J. Irwin, S.M. Barnett and D.L. Freeman, "Quantum Mechanical Studies of Local Water Structure Near Fixed Ions in Ion Exchange Membranes," *J. Membrane Sci.* **47**, 79 (1989).
34. C. Zhang, D.L. Freeman and J.D. Doll, "Monte Carlo Studies of Hydrogen Fluoride Clusters: Cluster Size Distributions in Hydrogen Fluoride Vapor," *J. Chem. Phys.* **91**, 2489 (1989).
35. J.D. Doll, T.L. Beck and D.L. Freeman, "Classical Monte Carlo Dynamics: A Simulated Annealing Approach to the Construction of Double Ended Classical Trajectories," *Int. J. Quant. Chem.*, **S23**, 73 (1989).
36. R.D. Coalson, D.L. Freeman and J.D. Doll, "Cumulant Methods and Short Time Propagators," *J. Chem. Phys.* **91**, 4242 (1989).
37. D.L. Freeman, T.L. Beck and J.D. Doll, "Stationary Phase Monte Carlo Evaluation of Direct Time Finite Temperature Dipole Autocorrelation Functions," in *Quantum Simulations of Condensed Matter Phenomena* (World Scientific, Teaneck, NJ, 1990), J.D. Doll and J.E. Gubernatis, Eds. p. 58

38. J.D. Doll, D.L. Freeman and T.L. Beck, "Equilibrium and Dynamical Fourier Path Integral Methods," *Adv. Chem. Phys.* **78**, 61 (1990).
39. D.D. Frantz, D.L. Freeman and J.D. Doll, "Reducing Quasi-Ergodic Behavior in Monte Carlo Simulations by J-Walking: Applications to Atomic Clusters," *J. Chem. Phys.* **93**, 2769 (1990).
40. J. Xie, J.A. Northby and D.L. Freeman, "A dynamical definition of atomic clusters," *J. Chem. Phys.* **95**, 3022 (1991).
41. S.W. Rick, D.L. Leitner, J.D. Doll, D.L. Freeman and D.D. Frantz, "The quantum mechanics of clusters: The low temperature equilibrium and dynamical behavior of rare gas systems," *J. Chem. Phys.*, **95**, 6658 (1991).
42. J.D. Doll, S.W. Rick and D.L. Freeman, "Stationary phase Monte Carlo Methods: Interference effects in Quantum Monte Carlo dynamics," *Can. J. Chem.*, **70**, 497 (1992).
43. M.A. Stozak, G.E. Lopez and D.L. Freeman, "Gibbs free-energy changes for the growth of argon clusters adsorbed on graphite," *J. Chem. Phys.*, **97**, 4445 (1992).
44. D.D. Frantz, D.L. Freeman and J.D. Doll, "Extending J-walking to quantum systems: Applications to atomic clusters," *J. Chem. Phys.*, **97**, 5713 (1992).
45. G.E. Lopez and D.L. Freeman, "A study of low temperature heat capacity anomalies in bimetallic alloy clusters using J- walking Monte Carlo methods," *J. Chem. Phys.*, **98**, 1428 (1993).
46. J.D. Doll and D.L. Freeman, "Monte Carlo methods in chemistry," *IEEE Computational Sci. Eng.*, **1**, 22 (1994).
47. D.L. Freeman and J.D. Doll, "Fourier path integral Monte Carlo method for the calculation of the microcanonical density of states," *J. Chem. Phys.*, **101**, 848 (1994).
48. J.D. Doll and D.L. Freeman, "Decisions, decisions: Noise and its effect on integral Monte Carlo algorithms," *Chem. Phys. Lett.* **227**, 436 (1994).
49. A.E. Cho, J.D. Doll and D.L. Freeman, "The construction of double-ended classical trajectories," *Chem. Phys. Lett.*, **229**, 218 (1994).
50. A. Matro, D.L. Freeman and J.D. Doll, "Locating transition states using double-ended classical trajectories," *J. Chem. Phys.*, **101**, 10458 (1994).
51. D.L. Freeman and J.D. Doll, "Computational studies of clusters: Methods and results," *Ann. Rev. Phys. Chem.*, **47**, 43 (1996).

52. A. Matro, D.L. Freeman and R.Q. Topper, "Computational study of the structure and thermodynamic properties of ammonium chloride clusters using a parallel j-walking approach," *J. Chem. Phys.*, **104**, 8690 (1996).
53. M. Eleftheriou, D. Kim, J.D. Doll and D.L. Freeman, "Information theory and the optimization of Monte Carlo simulations," *Chem. Phys. Lett.*, **276**, 353 (1997).
54. B. Chen, M.A. Gomez, M. Sehl, J.D. Doll and D.L. Freeman, "Theoretical studies of the structure and dynamics of metal/hydrogen systems: Diffusion and path integral Monte Carlo investigations of nickel and palladium clusters," *J. Chem. Phys.*, **105**, 9686 (1996).
55. J.D. Doll and D.L. Freeman, "Monte Carlo methods in chemistry: A tutorial," in *Modern Methods for Multidimensional Dynamics Computations in Chemistry*, D.L. Thompson, Editor, (World Scientific, New Jersey, 1998), pp 529-579
56. E. Curotto, A. Matro, D.L. Freeman and J.D. Doll, "A semi-empirical potential for simulations of transition metal clusters: Minima and isomers of  $Ni_n$  ( $n=2-13$ ) and their hydrides," *J. Chem. Phys.*, **108**, 729 (1998).
57. D. Kim, J.D. Doll and D.L. Freeman, "Dynamic path integral methods: A maximum entropy approach based on the combined use of real and imaginary time quantum Monte Carlo data," *J. Chem. Phys.*, **108**, 3871 (1998).
58. B. Chen, M.A. Gomez, J.D. Doll and D.L. Freeman, "Theoretical studies of the effect of hydrogen-hydrogen interactions on the structural and dynamical properties of metal/hydrogen clusters," *J. Chem. Phys.*, **108**, 4031 (1998).
59. E. Curotto, D.L. Freeman and J.D. Doll, "A j-walking algorithm for microcanonical simulations: Applications to Lennard-Jones clusters," *J. Chem. Phys.*, **109**, 1643 (1998).
60. E. Curotto, D.L. Freeman, B. Chen and J.D. Doll, "The melting transition of  $Ni_7$  and  $Ni_7H$  as modeled by a semi-empirical potential," *Chem. Phys. Lett.*, **295**, 366 (1998).
61. J.D. Doll, D. Kim, M. Eleftheriou, B. Chen, C. Bae and D.L. Freeman, "The Quantum Dynamics of Interfacial Hydrogen in Metals: An Introduction," in *Classical and Quantum Dynamics in Condensed Phase Simulations*, B. J. Berne, G. Ciccotti, and D. F. Coker editors, page 669 (World Scientific, River Edge, NJ, 1998)
62. M.A. Gomez, B. Chen, D.L. Freeman and J.D. Doll, "Quantum mechanics of hydrogen on nickel and palladium clusters," in *Theory of Atomic and Molecular Clusters*, J. Jellinek, Ed., (Springer-Verlag, Berlin, 1999), pp 309-325.
63. M. Eleftheriou, J.D. Doll, E. Curotto and D.L. Freeman, "The asymptotic convergence rates of Fourier path integral methods," *J. Chem. Phys.*, **110**, 6657 (1999).

64. J.D. Doll, M. Eleftheriou, S.A. Corcelli and D.L. Freeman, "Equilibrium and dynamical path integral methods," in *Quantum Monte Carlo Methods in Physics and Chemistry*, C. Umrigar and M.P. Nightingale, editors (Kluwer, Dordrecht, 1999), p. 213.
65. J.D. Doll and D.L. Freeman, "Comment on 'A comparison of the efficiency of Fourier and discretized path integral Monte Carlo'," *J. Chem. Phys.*, **111**, 7685 (1999).
66. D.B. Faken, A.F. Voter, D.L. Freeman and J.D. Doll, "Dimensional strategies and the minimization problem: Barrier avoiding algorithms," *J. Phys. Chem.* **A103**, 9521 (1999).
67. J.P. Neirotti, D.L. Freeman and J.D. Doll, "A heat capacity estimator for Fourier path integral simulations," *J. Chem. Phys.*, **112**, 3990 (2000).
68. D. Sabo, J.D. Doll and D.L. Freeman, "Self-adaptive quadrature and numerical path integration," *J. Chem. Phys.*, **113**, 2522 (2000).
69. J.P. Neirotti, F. Calvo, D.L. Freeman and J.D. Doll, "Phase changes in 38 atom Lennard-Jones clusters. I: A parallel tempering study in the canonical ensemble," *J. Chem. Phys.*, **112**, 10340 (2000)
70. F. Calvo, J.P. Neirotti, D.L. Freeman and J.D. Doll, "Phase changes in 38 atom Lennard-Jones clusters. II: A parallel tempering study of equilibrium and dynamic properties in the molecular dynamics and microcanonical ensembles," *J. Chem. Phys.*, **112**, 10350 (2000)
71. C. Bae, D.L. Freeman, J.D. Doll, G. Kresse and J. Hafner, "Energetics of hydrogen chemisorbed on Cu(110): A first principles calculations study," *J. Chem. Phys.*, **113**, 6926 (2000).
72. J.P. Neirotti, D.L. Freeman and J.D. Doll, "Approach to ergodicity in Monte Carlo simulations," *Phys. Rev. E*, **62**, 7445 (2000).
73. D. Sabo, J.D. Doll and D.L. Freeman, "Stationary tempering and the complex quadrature problem," *J. Chem. Phys.*, **116**, 3509 (2002).
74. A.E. Cho, J.D. Doll and D.L. Freeman, "Wavelet formulation of path integral Monte Carlo," *J. Chem. Phys.*, **117**, 5971 (2002).
75. R.Q. Topper, D.L. Freeman, D. Bergin and K.R. LaMarche, "Computational techniques and strategies for Monte Carlo thermodynamic calculations, with applications to nanoclusters," *Reviews in Computational Chemistry*, K. B. Lipkowitz, R. Larter, and T.R. Cundari, Eds., Wiley-VCH, Hoboken, NJ, 2003, Vol. 19, pp. 1-41
76. D. Sabo, J.D. Doll and D.L. Freeman, "Taming the rugged landscape: Techniques for the production, reordering and stabilization of selected cluster inherent structures," *J. Chem. Phys.*, **118**, 7321 (2003).

77. C. Predescu, D. Sabo, J.D. Doll and D.L. Freeman, "Energy estimators for random series path-integral methods," *J. Chem. Phys.*, **119**, 10475 (2003).
78. C. Predescu, D. Sabo, J.D. Doll and D.L. Freeman, "Heat capacity estimators for random series path-integral methods by finite-difference," *J. Chem. Phys.*, **119**, 12119 (2003).
79. D. Sabo, J.D. Doll and D.L. Freeman, "Monte Carlo Methods for Real Time Integration," in *The Monte Carlo Method in the Physical Sciences*, J. Gubernatis, ed., (American Institute of Physics Conference Proceedings, volume 690, Melville, NY (2003)), 396-397.
80. P. Nigra, D.L. Freeman, D. Sabo and J.D. Doll, "On the encapsulation of nickel clusters by molecular nitrogen," *J. Chem. Phys.*, **121**, 475 (2004).
81. D. Sabo, J.D. Doll and D.L. Freeman, "Taming the rugged landscape: Production, reordering and stabilization of selected cluster inherent structures in the  $X_{13-n}Y_n$  system," *J. Chem. Phys.*, **121**, 847 (2004).
82. D. Sabo, C. Predescu, J.D. Doll and D.L. Freeman, "Phase changes in selected Lennard-Jones  $X_{13-n}Y_n$  clusters," *J. Chem. Phys.*, **121**, 856 (2004).
83. C.V. Diaconu, A.E. Cho, J.D. Doll and D.L. Freeman, "Broken-symmetry unrestricted hybrid density functional calculations on nickel dimer and nickel hydride," *J. Chem. Phys.*, **121**, 10026 (2004).
84. D. Sabo, D.L. Freeman and J.D. Doll, "Pressure dependent study of the solid-solid phase change in 38-atom Lennard-Jones cluster," *J. Chem. Phys.*, **122**, 094716 (2005).
85. P. Nigra, D.L. Freeman and J.D. Doll, "Combining smart darting with parallel tempering using Eckart space: Application to Lennard-Jones clusters," *J. Chem. Phys.*, **122**, 114113 (2005)
86. S.F. Langley, E. Curotto, D.L. Freeman and J.D. Doll, "Rigid quantum Monte Carlo simulations of condensed molecular matter: Water clusters in the  $n = 2 \rightarrow 8$  range," *J. Chem. Phys.*, **126**, 084506 (2007).
87. D. Sabo, M. Meuwly, D.L. Freeman and J.D. Doll, "A constant entropy increase model for the selection of parallel tempering ensembles," *J. Chem. Phys.*, **128**, 174109 (2008).
88. E. Curotto, D.L. Freeman and J.D. Doll, "A stereographic projection path integral study of the coupling between the orientation and the bending degrees of freedom in water," *J. Chem. Phys.*, **128**, 204107 (2008).
89. N. Plattner, T. Bandi, J.D. Doll, D.L. Freeman and M. Meuwly, "MD simulations using distributed multipole electrostatics: Structural and spectroscopic properties of CO- and methane-containing clathrates," *Mol. Phys.*, **106**, 1675 (2008).

90. S. Kuniyev, D.L. Freeman and J.D. Doll, "A numerical study of the asymptotic convergence characteristics of partial averaged and reweighted Fourier path integral methods," *Int. J. Quant. Chem.*, **109**, 2916 (2009)
91. E. Asare, A. Musah, E. Curotto, D.L. Freeman and J.D. Doll, "The thermodynamic and ground state properties of the TIP4P water octamer," *J. Chem. Phys.*, **131**, 184508, (2009).
92. S.W. Rick and D.L. Freeman, "Proton disorder and the dielectric constant of type II clathrate hydrates," *J. Chem. Phys.*, **132**, 054509 (2010).
93. S.D. Kuniyev, D.L. Freeman and J.D. Doll, "Convergence characteristics of the cumulant expansion for Fourier path integrals," *Phys. Rev. E*, **81**, 066707 (2010).
94. G.L. Holden and D.L. Freeman, "Monte Carlo investigation of the thermodynamic properties of  $(\text{H}_2\text{O})_n$  and  $(\text{H}_2\text{O})_n\text{H}_2$  ( $n = 2 - 20$ ) clusters," *J. Phys. Chem. B*, **115**, 4725 (2011).
95. N. Plattner, S. Kuniyev, D.L. Freeman and J.D. Doll, "Numerical investigation of the cumulant expansion for Fourier path integrals," *PARA 2010, Part II, LNCS (Lecture Notes in Computer Science)* 7134, 13 (2012).
96. J.D. Doll, N. Plattner, D.L. Freeman, Y.i Liu, and P. Dupuis, "Rare-Event Sampling: Occupation-Based Performance Measures for Parallel Tempering and Infinite Swapping Monte Carlo Methods," *J. Chem. Phys.*, **137**, 204112 (2012).
97. B. Ruekberg and D.L. Freeman, "A(nother) modification of the ammonia fountain experiment," *J. Chem. Ed.*, **94** 1397 (2017).
98. B. Ruekberg and D.L. Freeman, "Elephant's Toothpaste Used as a Qualitative Demonstration of Rate versus Temperature," *J. Chem. Ed.*, **97**, 1061 (2020).

## Books

1. F.E. Harris, H.J. Monkhorst and D.L. Freeman, *Algebraic and Diagrammatic Methods in Many-Fermion Theory* (Oxford University Press, New York, 1992)
2. F.E. Harris, H.J. Monkhorst and D.L. Freeman, *Algebraic and Diagrammatic Methods in Many-Fermion Theory* (Dover Books, 2020)