

**Publication List**  
**ROB DUNCAN COALSON**

**PERSONAL DATA**

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**EDUCATION**

A.B. Degree:	Physics and Chemistry, Harvard University, 1977
Ph.D:	Chemical Physics, Harvard University, 1984
Director's Funded Postdoctoral Fellow:	Los Alamos National Laboratory, 1984-1986

**Honors:** A.B., magna cum laude  
Phi Beta Kappa  
NSF Presidential Young Investigator, 1986-1991  
Alfred P. Sloan Research Fellow, 1988-90  
Camille and Henry Dreyfus Teacher Scholar, 1989-94  
Fellow, Institute for Advanced Studies, Hebrew University of Jerusalem, 1993  
NSF Special Creativity Extension Award, 1993-95  
Chancellor's Distinguished Research Award (Junior Scholar Category),  
University of Pittsburgh, 1995  
Fellow, Japanese Society for the Promotion of Science, 1996  
Fellow, American Physical Society, 1999  
Chancellor's Distinguished Research Award (Senior Scholar Category),  
University of Pittsburgh, 2006

Thesis Title: Time-dependent Quantum Mechanical Techniques for the Study of Molecular Processes

Thesis Advisor: Professor Martin Karplus

**PUBLICATIONS**

1. "Extended Wavepacket Dynamics: Exact Solution for Collinear Atom, Diatomic Molecule Scattering", R. D. Coalson and M. Karplus, Chem. Phys. Lett., **90**, 301 (1982).
2. "Generalized Quantum Liouville Equation: Its Solution by Wave Packet Dynamics", R. D. Coalson and M. Karplus, J. Chem. Phys., **79**, 6150 (1983).

3. "Inclusion of Frequency Shifts in the Treatment of N-Photon Vibronic Processes Involving Uncoupled Harmonic Surfaces: A Simple and Exact Prescription", R. D. Coalson, *J. Chem. Phys.*, **81**, 2794 (1984).
4. "New Sum Rules for Electronic Absorption Spectra", R. D. Coalson and M. Karplus, *J. Chem. Phys.*, **81**, 2891 (1984).
5. "On the Computation of two Surface Propagators via Coordinate Space Propagator Techniques", R. D. Coalson, *J. Chem. Phys.*, **83**, 688 (1985).
6. "A Partial Averaging Prescription for Fourier Path Integrals", J. D. Doll, R. D. Coalson, and D. L. Freeman, *Phys. Rev. Lett.*, **55**, 1 (1985).
7. "Fourier Path Integral Methods: A Model Study for Simple Fluids", D. L. Freeman, R. D. Coalson, and J. D. Doll, *J. Stat. Phys.*, **43**, 931 (1986).
8. "On the Connection Between Fourier Coefficient and Discretized Cartesian Path Integration", R. D. Coalson, *J. Chem. Phys.*, **85**, 926 (1986).
9. "Partial Averaging Approach to Fourier Coefficient Path Integration", R. D. Coalson, D. L. Freeman, and J. D. Doll, *J. Chem. Phys.*, **85**, 4567 (1986).
10. "Time Domain Formulation of Optical Spectroscopy Involving Three Potential Surfaces", R. D. Coalson and J. L. Kinsey, *J. Chem. Phys.*, **85**, 4322 (1986).
11. "Emission Spectroscopy of Photodissociating Molecules: A Collinear Model for CH<sub>3</sub>I and CD<sub>3</sub>I", R. L. Sundberg, D. Imre, M. O. Hale, J. L. Kinsey, and R. D. Coalson, *J. Phys. Chem.*, **90**, 5001 (1986).
12. "A Spin-Boson Model for Spectroscopy Involving Nonadiabatically Coupled Potential Energy Surfaces", R. D. Coalson, *J. Chem. Phys.*, **86**, 995 (1987).
13. "Time-Domain Formulation of Photofragmentation Involving Nonradiatively Coupled Excited States, and its Implementation via Wave Packet Perturbation Theory", R. D. Coalson, *J. Chem. Phys.*, **86**, 6823 (1987).
14. "Towards a Monte Carlo Theory of Quantum Dynamics", J. D. Doll, R. D. Coalson, and D. L. Freeman, *J. Chem. Phys.*, **87**, 1641 (1987).
15. "Dynamic Aspects of Electronic Excitation", M. V. Rama Krishna and R. D. Coalson, *Chem. Phys.*, **120**, 327 (1988).
16. "Time-Domain Theory for Computing Excited State Optical Lineshapes Induced by Nonradiative Coupling in the Single Bright State Approximation", R. D. Coalson, *Chem. Phys. Lett.*, **147**, 208 (1988).
17. "Time-Dependent Wavepacket Approach to Optical Spectroscopy Involving Nonadiabatically Coupled Potential Surfaces", R. D. Coalson, *Adv. Chem. Phys.*, **73**, 605 (1989).

18. "Time-Dependent Hartree Wavepacket Dynamical Techniques for Computation of Electronically Excited State Optical Spectra of Many-body Quantum Systems", M. Messina and R. D. Coalson, *J. Chem. Phys.*, **90**, 4015 (1989).
19. "Spectroscopic Spin-Boson Model in the Adiabatic Limit: Application to Optical Lineshapes", R. D. Coalson, *Phys. Rev. B*, **39**, 12052 (1989).
20. "Cumulant Methods and Short Time Propagators", R. D. Coalson and D. L. Freeman, and J. D. Doll, *J. Chem. Phys.*, **91**, 4242 (1989).
21. "Application of the Time Dependent Hartree Grid Method to Inelastic Molecular Scattering Problems", R. D. Coalson, *Chem. Phys. Lett.*, **165**, 443 (1990).
22. "Computation of Spectroscopic Observables for Condensed Phase Systems", M. Messina and R. D. Coalson, in Quantum Simulations of Condensed Matter, J. D. Doll and J. E. Gubernatis, Eds. pp. 203-227, (World Scientific, 1990).
23. "Extended Adiabatic Formalism for Computing Thermodynamic Properties of a Quantum System Coupled to a Nonadiabatic Bosonic Bath", R. D. Coalson, *J. Chem. Phys.*, **92**, 4993 (1990).
24. "Time-of-Flight Spectra of a Particle Scattering from a Collinear Harmonic Lattice at Finite Temperature", M. Messina and R. D. Coalson, *J. Chem. Phys.*, **92**, 5297 (1990).
25. "Reduced Partial Dissociation Cross Sections for a Molecule Photodesorbed from a Surface", M. Messina and R. D. Coalson, *J. Chem. Phys.*, **92**, 5712, (1990).
26. "Multidimensional Variational Gaussian Wavepacket Dynamics with Application to Photodissociation Spectroscopy", R. D. Coalson and M. Karplus, *J. Chem. Phys.*, **93**, 3919 (1990).
27. "Adding Configuration Interaction to the Time-dependent Hartree Grid Approximation", J. Campos-Martinez and R. D. Coalson, *J. Chem. Phys.*, **93**, 4740 (1990).
28. "Obtaining Long-time Dynamics in the Spectroscopic Spin-Boson Model via Path Integration", R. D. Coalson, *J. Chem. Phys.*, **94**, 1108 (1991).
29. "Application of a Coupled-Surface Time-Dependent Hartree Grid Method to Excited State Optical Spectroscopy", J. R. Waldeck, J. Campos-Martinez, and R. D. Coalson, *J. Chem. Phys.*, **94**, 2773 (1991).
30. "A Wavepacket Golden Rule Treatment of Vibrational Predissociation", P. Villarreal, S. Miret-Artes, O. Roncero, G. Delgado-Barrio, J. A. Beswick, N. Halberstadt, and R. D. Coalson, *J. Chem. Phys.*, **94**, 4230 (1991).
31. "Reduced Partial Cross Sections for UV Photodesorption of Molecules From Finite Temperature Surfaces", M. Messina and R. D. Coalson, *J. Chem. Phys.*, **95**, 5364 (1991).
32. "Time of Flight Spectra and Angular Observables for U.V. Photodesorption of Molecules from Surfaces", M. Messina and R. D. Coalson, *J. Chem. Phys.*, **95**, 8977 (1991).

33. "Beyond the Time-Dependent Hartree Grid Approximation for Curve-Crossing Problems", J. Campos-Martinez, J. R. Waldeck and R. D. Coalson, *J. Chem. Phys.*, **96**, 3613 (1992).
34. "Melting of Colloidal Crystals: A Monte Carlo Study", J. C. Zahorchak, R. Kesavamoorthy, R. D. Coalson, and S. A. Asher, *J. Chem. Phys.*, **96**, 6873 (1992).
35. "Using Relaxation Theory to Compute the Electronic Absorption Spectrum of a Chromophore Coupled to a Condensed Phase Environment", D. G. Evans and R. D. Coalson, *J. Chem. Phys.*, **97**, 5081 (1992).
36. "Systematic Ionic Screening Theory of Macroions", R. D. Coalson and A. Duncan, *J. Chem. Phys.*, **97**, 5653-61 (1992).
37. "Redfield Theory is Quantitative for Coupled Harmonic Oscillators," A. M. Walsh and R. D. Coalson, *Chem. Phys. Lett.*, **198**, 293 (1992).
38. "Relaxation Theory for Curve-Crossing Corrections to Electronic Absorption Line Shapes in Condensed Phases", D. G. Evans and R. D. Coalson, *J. Chem. Phys.*, **99**, 6264 (1993).
39. "Application of the TDHG-CI Method to the Desorption of Diatomic Molecules from Solid Surfaces", J. Campos-Martinez and R. D. Coalson, *J. Chem. Phys.*, **99**, 9629 (1993).
40. "Lattice Field Theory for Spherical Macroions in Solution: Calculation of Equilibrium Pair Correlation Functions", A. M. Walsh and R. D. Coalson, *J. Chem. Phys.*, **100**, 1559-66 (1994).
41. "System-Bath Relaxation Theory Approach to Curve-Crossing Effects on Condensed Phase Electronic Absorption Spectra", D. G. Evans and R. D. Coalson, *J. Chem. Phys.*, **100**, 5605 (1994).
42. "Life-times of Selective Adsorption Resonances in Atom-Surface Elastic Scattering", M. I. Hernandez, J. Campos-Martinez, S. Miret-Artes and R. D. Coalson, *Phys. Rev. B.*, **49**, 8300 (1994).
43. "A Nonequilibrium Golden Rule Formula for Electronic State Populations in Nonadiabatically Coupled Systems", R. D. Coalson, D. G. Evans and A. Nitzan, *J. Chem. Phys.*, **101**, 436 (1994).
44. "Computing the Eigenmodes of Lossy Field-Induced Optical Waveguides", R. D. Coalson, D. K. Pant, A. Ali and D. W. Langer, *J. Lightwave Tech.*, **12**, 1015 (1994).
45. "Dielectric Constant Effects on the Energetics of Oppositely Charged Colloids. A Lattice Field Theory Study", N. Ben-Tal and R. D. Coalson, *J. Chem. Phys.*, **101**, 5148 (1994).
46. "Statistical Mechanics of a Coulomb Gas with Finite Size Particles: A Lattice Field Theory Approach", R. D. Coalson, A. M. Walsh, A. Duncan and N. Ben-Tal, *J. Chem. Phys.*, **102**, 4584-94 (1995).
47. "Incorporating Backflow into a Relaxation Theory Treatment of the Dynamics of Nonequilibrium Nonadiabatic Transition Process", D. G. Evans and R. D. Coalson, *J. Chem. Phys.*, **102**, 5658-68 (1995).

48. "Manipulating Reactant-Product Distributions in Electron Transfer Reactions with a Laser Field", R. D. Coalson and Y. Dakhnovskii, *J. Chem. Phys.*, **103**, 2908-16 (1995).
49. "The Effect of a Laser Field on Electron Transfer in Metal Complexes: Quantum Degrees of Freedom", Y. Dakhnovskii, D. G. Evans, H. J. Kim and R. D. Coalson, *J. Chem. Phys.*, **103**, 5461-69 (1995).
50. "Inducing Coherent Oscillations in the Electron Transfer Dynamics of a Strongly Dissipative System with Pulsed Monochromatic Light", D. G. Evans, R. D. Coalson, H. J. Kim and Y. Dakhnovskii, *Phys. Rev. Lett.*, **75**, 3649-52 (1995).
51. "Induced Oscillations in an Electron Transfer Reaction in the Presence of a Bichromatic Electromagnetic Field", D. G. Evans, R. D. Coalson and Y. Dakhnovskii, *J. Chem. Phys.*, **104**, 2287-96 (1996).
52. "Simulation of Electron Transfer in Polar Solvents: Effects of Nonequilibrium Initial State Preparation", D. G. Evans and R. D. Coalson, *J. Chem. Phys.*, **104**, 3598-3608 (1996).
53. "Statistical Mechanics of a Multipolar Gas: A Lattice Field Theory Approach", R. D. Coalson and A. Duncan, *J. Phys. Chem.*, **100**, 2612-20 (1996).
54. "A Wavepacket-Path Integral Method for Curve Crossing Dynamics", R. D. Coalson, *J. Phys. Chem.*, **100**, 7896-7902 (1996).
55. "A Molecular Dynamics Study of Dielectric Friction", M. G. Kurnikova, D. H. Waldeck and R. D. Coalson, *J. Chem. Phys.*, **105**, 628-38 (1996).
56. "Laser Control of Polar Electron Transfer Dynamics", R. D. Coalson, D. G. Evans and Y. Dakhnovskii, in *Femtochemistry: Ultrafast Chemical and Physical Processes in Molecular Systems*, M. Chergui, Ed., pp. 338-47 (World Scientific, 1996).
57. "Nonadiabatic Dynamics and Electronic Energy Relaxation of  $\text{Cl}(^2P)$  Atoms in Solid Ar", A. I. Krylov, R. B. Gerber and R. D. Coalson, *J. Chem. Phys.*, **105**, 4626-35 (1996).
58. "Light Absorption in Strongly Irradiated Long Range Polar Electron Transfer Systems", Y. Dakhnovskii, V. Lubchenko and R. D. Coalson, *Phys. Rev. Lett.*, **77**, 2917-20 (1996).
59. "Multiphoton Absorption by Metal-Metal Long Distance Charge Transfer Complexes in Polar Solvents", Y. Dakhnovskii, V. Lubchenko and R. D. Coalson, *J. Chem. Phys.*, **105**, 9441-53 (1996).
60. "A Molecular Dynamics Study of Photothermal Compression of Colloidal Crystals", J. C. Zahorchak, M. G. Kurnikova and R. D. Coalson, *J. Chem. Phys.*, **106**, 1585-92 (1997).
61. "A Wavepacket-Path Integral Method for Curve-crossing Problems: Application to Resonance Raman Spectra and Photodissociation Cross Sections", A. E. Cárdenas and R. D. Coalson, *Chem. Phys. Lett.*, **265**, 71-76 (1997).
62. "Design and Analysis of Wide-Angle Y-Branch Waveguide with Low-Losses for Integrated Optics", D-S Min, D. W. Langer, D. K. Pant, and R. D. Coalson, *SPIE Proceedings*, **3006**, 459 (1997).
63. "Wide-Angle Low-Loss Waveguide Branching for Integrated Optics", D. S. Min, D. W. Langer, D. K. Pant, and R. D. Coalson, *Fiber and Integrated Optics*, **16**, 331-42 (1997).

64. "Optimal Control Theory for the Design of Optical Waveguides", D. K. Pant, R. D. Coalson, M. I. Hernández and J. Campos-Martínez, *J. Lightwave Tech.*, **16**, 292-300 (1998).
65. "Numerical Methods for Solving Poisson and Poisson-Boltzmann Type Equations", R. D. Coalson and T. L. Beck, *Encyclopedia of Computational Chemistry* (Wiley), P. von Rague Schleyer, ed., Vol. 3, pp. 2086-2100 (1998).
66. "Rotational Relaxation in Polar Solvents. Molecular Dynamics Study of Solute—Solvent Interaction", M. G. Kurnikova, N. Balabai, D. H. Waldeck, and R. D. Coalson, *J. Am. Chem. Soc.*, **120**, 6121-30 (1998).
67. "Long-Range Electron Transfer Driven by Two Lasers: Induced Irradiance", Y. Dakhnovskii, V. Lubchenko and R. D. Coalson, *J. Chem. Phys.*, **109**, 691-703 (1998).
68. "Rotational Diffusion of Organic Solutes: The Role of Dielectric Friction in Polar Solvents and Electrolyte Solutions", N. Balabai, A. Sukharevsky, I. Read, B. Straszisar, M. Kurnikova, R. S. Hartman, D. H. Waldeck and R. D. Coalson, *J. Mol. Liquids*, **77**, 37-60(1998).
69. "Rotational Relaxation of Ionic Molecules in Electrolyte Solutions: Anisotropy Relaxation and Molecular Dynamics Study", N. Balabai, M. Kurnikova, R. D. Coalson, and D. H. Waldeck, *J. Am. Chem. Soc.*, **120**, 7944-51 (1998).
70. "A Lattice Relaxation Algorithm for 3D Poisson-Nernst-Planck Theory with Application to Ion Transport Through the Gramicidin A Channel", M. Kurnikova, R. D. Coalson, P. Graf, and A. Nitzan, *Biophys. J.*, **76**, 642-56 (1999).
71. "Entropic Trapping of a Flexible Polymer in a Fixed Network of Random Obstacles", S-S. Chern and R. D. Coalson, *J. Chem. Phys.*, **111**, 1778-81 (1999).
72. "Optimal Control Theory for Optical Waveguide Design: Application to Y-branch Structures", D. K. Pant, R. D. Coalson, M. I. Hernández and J. Campos-Martínez, *Appl. Op.*, **38**, 3917-23 (1999).
73. "Calculation of Reduced Partial Cross Sections of Molecules Photodesorbing from a Cold Crystal Surface with Internal Vibrations: Inclusion of Curve-Crossing Effects", A. E. Cárdenas and R. D. Coalson, *J. Chem. Phys.*, **110**, 11542-50 (1999).
74. "Statistical Mechanics of Charged Polymers in Electrolyte Solutions: A Lattice Field Theory Approach", S. Tsonchev, R. D. Coalson, and A. Duncan, *Phys. Rev. E*, **60**, 4257-67 (1999).
75. "Semiclassical Wave Packet Dynamics with Electronic Structure Computed on the Fly: Application to Photophysics of Electronic Excited States in Condensed Phase", A. E. Cárdenas, R. Krems, and R. D. Coalson, *J. Phys. Chem. A*, **103**, 9469-74 (1999).
76. "A Theoretical Description of Microdialysis with Mass Transport Coupled to Chemical Events", H. Yang, J. L. Peters, C. Allen, S.-S. Chern, R. D. Coalson, and A. C. Michael, *Anal. Chem.*, **72**, 2042-2049 (2000).
77. "3D Poisson-Nernst-Planck Theory Studies: Influence of Membrane Electrostatics on Gramicidin A Channel Conductance", A. E. Cárdenas, R. D. Coalson and M. G. Kurnikova, *Biophys. J.*, **79**, 80-93 (2000).
78. "Partitioning of a Polymer Chain Between Two Confining Cavities: The Role of Electrostatic

- Interactions", S. Tsonchev, R. D. Coalson and A. Duncan, *Phys. Rev. E*, **62**, 799-806 (2000).
79. "Partitioning of a Polymer Chain Between Two Confining Cavities: The Roles of Excluded Volume and Finite Size Conduits", S. Tsonchev and R. D. Coalson, *Chem. Phys. Lett.*, **327**, 238-244 (2000).
  80. "On the Reliability of Mean-Field Methods in Polymer Statistical Mechanics", S. Tsonchev, R. D. Coalson, S-S. Chern and A. Duncan, *J. Chem. Phys.*, **113**, 8381-8389 (2000).
  81. "A Dynamic Lattice Monte Carlo Model of Ion Transport in Inhomogeneous Dielectric Environments: Method and Implementation", P. Graf, A. Nitzan, M. G. Kurnikova and R. D. Coalson, *J. Phys. Chem. B*, **104**, 12324-12338 (2000).
  82. "3D Dynamic Monte Carlo Simulations of Driven Polymer Transport Through a Hole in a Wall", S-S. Chern, A. E. Cárdenas, and R. D. Coalson, *J. Chem. Phys.*, **115**, 7772-7773 (2001).
  83. "Control of Electron Current by Double-Barrier Structures using Pulsed Laser Fields", J. T. York, R. D. Coalson, and Y. Dahnovsky, *Phys. Rev. B*, **65**, 235321 (2002).
  84. "Calculating Electron Transport in a Tight-Binding Model of a Field-Driven Molecular Wire: Floquet Theory Approach", A. Tikhonov, R. D. Coalson, and Y. Dahnovsky, *J. Chem. Phys.*, **116**, 10909-10920 (2002).
  85. "Calculating Electron Current in a Tight-Binding Model of a Field-Driven Molecular Wire: Application to Xylyl-dithiol", A. Tikhonov, R. D. Coalson, and Y. Dahnovsky, *J. Chem. Phys.*, **117**, 567-580 (2002).
  86. "The Role of the Dielectric Barrier in Narrow Biological Channels: a Novel Composite Approach to Modeling Single Channel Currents", A. Mamonov, R. D. Coalson, A. Nitzan, and M. G. Kurnikova, *Biophys. J.*, **84**, 3646-3661 (2003).
  87. "The Wide-Angle Equation and its Solution through the Short Time Iterative Lanczos Method", J. Campos-Martinez and R. D. Coalson, *Appl. Optics*, **42**, 1732-1742 (2003).
  88. "Condensed Phase Vibrational Relaxation: Calibration of Approximate Relaxation Theories with Analytical and Numerically Exact Results", R. D. Coalson and D. G. Evans, *Chem. Phys.*, **296**, 117-127 (2004).
  89. "Comparison of Dynamic Lattice Monte-Carlo Simulations and Dielectric Self Energy Poisson-Nernst-Planck Continuum Theory for Model Ion Channels", P. Graf, M.G. Kurnikova, R. D. Coalson and A. Nitzan, *J. Phys. Chem. B*, **108**, 2006-2015 (2004).
  90. "Crystalline Colloidal Array Photonic Crystal Diffraction", S.A. Asher, J.M. Weissman, A. Tikhonov, R.D. Coalson and R. Kesavamoorthy, *Phys. Rev. E*, **69**, 066619:1-14 (2004)
  91. "Flexible Polyelectrolyte Simulations at the Poisson-Boltzmann Level: a Comparison of the Kink-Jump and Multigrid Configurational-Bias Monte Carlo Methods", S. Tsonchev, R. D. Coalson, A. Liu and T. L. Beck, *J. Chem. Phys.*, **120**, 9817-9821 (2004).
  92. "Collective Properties of Indirect Excitons in Coupled Quantum Wells in a Random Field", O. L. Berman, Yu. E. Lozovik, D. W. Snoke, and R. D. Coalson, *Phys. Rev. B*, **70**, 235310:1-8 (2004).
  93. "An Accurate and Efficient Empirical Approach for Calculating the Dielectric Self Energy and Ion-ion Pair Potential in Biological Ion Channels", M. H. Cheng and R. D. Coalson, *J. Phys.*

- Chem. B, **109**, 488-498 (2005).
94. "Superfluidity of 'Dirty' Indirect Excitons in Coupled Quantum Wells". O. L. Berman, Yu. E. Lozovik, D. W. Snoke, and R. D. Coalson, *Solid State Comm.*, **134**, 47-50 (2005).
  95. "Poisson-Nernst-Planck Theory Approach to the Calculation of Current through Biological Ion Channels", R. D. Coalson and M. G. Kurnikova, *IEEE Trans. on Nanobio.*, **4**, 81-93 (2005).
  96. "Improved Local Lattice Approach for Coulombic Simulations", A. Duncan, R. D. Sedgewick, and R. D. Coalson, *Phys. Rev. E*, **71**, 046702:1-8 (2005)
  97. "Theoretical Studies of the M2 Transmembrane Segment of the Glycine Receptor: Models of the Open Pore Structure and Current-Voltage Characteristics", M. H. Cheng, M. Cascio, and R. D. Coalson, *Biophys. J.*, **89**, 1669-1680 (2005). [Note: This work was featured on the cover of the *Biophysical Journal*, Sept. 2005 issue: [www.biophysj.org/content/vol89/issue3/cover.shtml](http://www.biophysj.org/content/vol89/issue3/cover.shtml) .]
  98. "The Band Structure of Photonic Band-Gap Crystals with Superconducting Elements", O. L. Berman, Yu. E. Lozovik, S. L. Eiderman, and R. D. Coalson, *AIP Conference Proceedings* **850**, Part A, 997-998 (2006).
  99. "Exact Solution of a Model of Condensed-Phase Electron Transfer with Non-Condon Effects", W. R. Cook, D. G. Evans, and R. D. Coalson, *Chem. Phys. Lett.*, **420**, 362–366 (2006).
  100. "A Rigid-Body Newtonian Propagation Scheme based on Instantaneous Decomposition into Rotation and Translation Blocks", S. Essiz and R. D. Coalson, *J. Chem. Phys.*, **124**, 144116:1-11 (2006).
  101. "Local Simulation Algorithms for Coulomb Gases with Dynamical Dielectric Effects", A. Duncan, R. D. Sedgewick, and R. D. Coalson, *Phys. Rev. E*, **73**, 016705:1-6 (2006).
  102. "Poisson-Nernst-Planck Theory of Ion Permeation through Biological Channels", R. D. Coalson and M. G. Kurnikova, in *Biological Membrane Ion Channels: Dynamics, Structure, and Applications*, S-H. Chung, O. S. Andersen, and V. Krishnamurthy, Ed., 449-484 (Springer Science+Business Media, New York, 2007).
  103. "Fast Fourier Transform Simulation Techniques for Coulomb Gases", A. Duncan, R. D. Sedgewick, and R.,D. Coalson, *Comp.r Phys. Comm.*, **175**, 73-77 (2006).
  104. "An Introduction to Simulation and Visualization of Biological Systems at Multiple Scales: A Summer Training Program for Interdisciplinary Research", R. Munshi, R. D. Coalson, G. B. Ermentrout, J. D. Madura, H. Meirovitch, J. R. Stiles, and I. Bahar, *Biotechn. Progr.*, **22**, 179-185 (2006).
  105. "Diffusion Constant of K<sup>+</sup> inside Gramicidin A: a Comparative Study of Four Computational Methods", A. B. Mamonov, M. G. Kurnikova, and R. D. Coalson, *Biophys. Chem.*, **124**, 268-278 (2006).
  106. "Superfluidity of Dirty Indirect Excitons and Magnetoexcitons in a Two-dimensional Trap", O. L. Berman, Yu. E. Lozovik, D. W. Snoke, and R.D. Coalson, *Phys. Rev. B*, **73**, 235352:1-5 (2006).
  107. "Phase transitions of Indirect Excitons in Coupled Quantum Wells: The Role of Disorder", O. L. Berman, Yu. E. Lozovik, D. W. Snoke, and R. D. Coalson, *Physica E*, **32**, 1-612 (May 2006) [Proceedings of the 12th International Conference on Modulated Semiconductor



Structures.]

- 108 "Condensed-phase Relaxation of Multilevel Quantum Systems. I. An Exactly Solvable Model", S. Peter, D. G. Evans, and R. D. Coalson, *J. Phys. Chem. B*, **110**, 18758-18763 (2006).
- 109 "Condensed-phase Relaxation of Multilevel Quantum Systems. II. "Comparison of Path Integral Calculations and Second-Order Relaxation Theory for a Non-degenerate Three-level System", S. Peter, D.G. Evans, and R.D. Coalson, *J. Phys. Chem. B*, **110**, 18764-18770 (2006).
110. "Unfolding of Alanine-based Peptides using Electron Spin Resonance Distance Measurements", S. Jun, J. S. Becker, M. Yonkunas, R. D. Coalson, and S. Saxena, *Biochem.*, **45**, 11666-11673 (2006).
- 111 "Superconducting Photonic Crystals: Numerical Calculations of the Band Structure", O. L. Berman, Yu. E. Lozovik, S. L. Eiderman, and R. D. Coalson, *Phys. Rev. B*, **74**, 092505:1-3 (2006).
112. "Homology Modeling and Molecular Dynamics Simulations of the  $\alpha 1$  Glycine Receptor Reveals Different States of the Channel", M. H. Cheng, M. Cascio, and R. D. Coalson, *Proteins: Structure, Function and Bioinformatics*, **68**, 581-593 (2007).
113. "Modeling the Fast Gating Mechanism in ClC Chloride Channels", M. H. Cheng, A. B. Mamonov, J. W. Dukes and R. D. Coalson, *J. Phys. Chem. B*, **111**, 5956-5965 (2007).
114. "Water and Deuterium oxide Permeability Through Aquaporin : MD Predictions and Experimental Verification", A. B. Mamonov, R. D. Coalson, M. L. Zeidel, and J. C. Mathai, *J. Gen. Phys.*, **130**, 111-116 (2007).
115. "Langevin Dynamics of Molecules with Internal Rigid Fragments in the Harmonic Regime", S. G. Essiz and R. D. Coalson, *J. Chem. Phys.* **127**, 104109:1-11 (2007).
116. "Superfluidity of 'dirty' Indirect Magnetoexcitons in Coupled Quantum Wells in High Magnetic Field", O. L. Berman, Y. E. Lozovik, D. W. Snoke ,and R. D. Coalson, *J. Phys: Condensed Matter* **19**, 386219:1-16 (2007).
117. "Partitioning of a Polymer Chain between a Confining Cavity and a Gel", S. Tsonchev, R.D. Coalson and A. Duncan, *Phys. Rev. E*, **76**, 041804:1-6 (2007)
118. "Discrete State Model of Coupled Ion Permeation and Fast Gating in ClC Chloride Channels", R. D. Coalson, *J. Phys. A*, **41**, 115001:1-15 (2008).
119. "Computational Prediction of Ion Permeation Characteristics in the Glycine Receptor Modified By Photo-Sensitive Compounds", M. H. Cheng, R. D. Coalson, M. Cascio, and M. Kurnikova, *J. Comp.-Aided Molec. Design*, **22**, 563-570 (2008).
120. "Molecular Dynamics Simulations of Ethanol Binding to the Transmembrane Domain of the Glycine Receptor: Implications for the Channel Potentiation Mechanism", M. H. Cheng, R. D. Coalson, and M. Cascio, *Proteins: Structure, Function and Bioinformatics*, **71**, 972-981 (2008).
121. "Light Diffraction from Modulated Colloidal Crystals with Low Dielectric Constant: Simulations Using Single-Scattering Theory", A. Tikhonov, R. D. Coalson, and S. A. Asher, *Phys. Rev. B*, **77**, 235404:1-16 (2008).
122. "*In Silico* Models for the Human  $\alpha 4\beta 2$  Nicotinic Acetylcholine Receptor", E. J. Haddadian,

- M. H. Cheng, R.D. Coalson, Y. Xu, and P.Tang, *J. Phys. Chem. B*, **112**, 13981-13990 (2008).
123. "Molecular Basis for Cation Selectivity in Claudin-2-based Paracellular Pores: Identification of an Electrostatic Interaction Site", A. S. L. Yu, M. H. Cheng, S. Angelow, D. Günzel, S. A. Kanzawa, E. E. Schneeberger, M. Fromm, and R. D. Coalson, *J. Gen. Phys.*, **133**, 111-127 (2009).
  124. "The Effectiveness of Perturbation Theory Approaches for Computing Non-Condon Electron Transfer Dynamics in Condensed Phases" W. R. Cook, R. D. Coalson, and D. G. Evans, *J. Phys. Chem. B*, **113**, 11437-11447 (2009).
  125. "Dynamic Linear Response Theory for Conformational Relaxation of Proteins", S. Essiz and R. D. Coalson, *J. Phys. Chem. B*, **113**, 10859-10869 (2009).
  126. "Discrete-State Representation of Ion Permeation Coupled to Fast Gating in a Model of ClC-Chloride Channels: Comparison to Multi-ion Continuous Space Brownian Dynamics Simulations", R.D. Coalson and M. H. Cheng, *J. Phys. Chem. B*, **114**, 1424–1433 (2010).
  127. "The electrostatics of VDAC: implications for selectivity and gating", O. P. Choudhary, R. Ujwal, W. Kowallis, R. D. Coalson, J. Abramson, and M. Grabe, *J. Mol. Biol.*, **396**, 580-592 (2010).
  128. "Calcium Inhibits Paracellular Sodium Conductance through Claudin-2 by Competitive Binding", A.S.L. Yu, M.H. Cheng and R.D. Coalson, *J. Biol. Chem.*, **285**, 37060-37069 (2010).
  129. "Molecular Dynamics and Brownian Dynamics Investigation of Ion Permeation and Anesthetic Halothane Effects on a Proton-Gated Ion Channel", M. H. Cheng, R.D. Coalson and P. Tang, *J. Am. Chem. Soc.*, **132**, 16442-16449 (2010).
  130. "Discrete-State Representation of Ion Permeation Coupled to Fast Gating in a Model of ClC-Chloride Channels: Analytic Estimation of the State-to-State Rate Constants", R.D. Coalson and M. H. Cheng, *J. Phys. Chem. A*, **115**, 9633–9642 (2011).
  131. "Molecular Dynamics Investigation of Cl<sup>-</sup> and Water Transport through a Eukaryotic CLC Transporter", M.H. Cheng and R.D. Coalson, *Biophys. J.*, **102**, 1363-1371 (2012).
  132. "Morphological control of grafted polymer films via attraction to small nanoparticle inclusions", M.G. Opferman, R.D. Coalson, D. Jasnow and A. Zilman, *Phys. Rev. E*, **86**, 031806:1-7 (2012) [A preliminary account of this work is given in M.G. Opferman, R.D. Coalson, D. Jasnow, and A. Zilman, *Morphological Control of Grafted Polymer Films by Nanoparticle Binding*, <http://arxiv.org/abs/1110.6419>, 2011.]
  133. "Response of Rotation–Translation Blocked Proteins Using Langevin Dynamics on a Locally Harmonic Landscape", A.C. Manson and R.D. Coalson, *J. Phys. Chem.*, **116**, 12142–12158 (2012).
  134. "Energetics and Ion Permeation Characteristics in a Glutamate-gated Chloride (GluCl) Receptor Channel", M.H. Cheng and R.D. Coalson, *J. Phys. Chem. B*, **116**, 13637–13643 (2012).
  135. "Metal Binding Sites of Human H-chain Ferritin and Iron Transport Mechanism to the

- Ferroxidase Sites: a Molecular Dynamics Simulation Study”, R. Laghaei, R.D. Coalson and D.G. Evans, *Proteins: Structure, Function, and Bioinformatics*, **81**, 1042-1050 (2013).
136. “Surface Plasmon Polaritons and Optical Transmission through a Vortex Lattice in a Film of Type-II Superconductor”, O. L. Berman, Y.E. Lozovik, A.A. Kolesnikov, M.V. Bogdanova, and R. D. Coalson, *J. Opt. Soc. Am. B*, **30**, 909-913 (2013).
  137. “Langevin Dynamics Simulation of 3D Colloidal Crystal Vacancies and Phase Transitions”, R. Laghaei, R.D. Coalson and S.A. Asher, *J. Phys. Chem. B*, **117**, 5271–5279 (2013)
  138. “Overdamped Dynamics of Folded Protein Domains within a Locally Harmonic Basin Using Coarse Graining based on a Partition of Compact Flexible Clusters”, A.C. Manson and R.D. Coalson, *J. Phys. Chem. B*, **117**, 6646–6655 (2013).
  139. “The Morphology of Polymer Brushes Infiltrated by Attractive Nanoinclusions of Various Sizes”, M.G. Opferman, R.D. Coalson, D. Jasnow and A. Zilman, *Langmuir*, **29**, 8584–8591 (2013).
  140. “Calculation of Iron Transport through Human H-chain Ferritin”, R. Laghaei, W. Kowallis, D.G. Evans and R.D. Coalson, *J. Phys. Chem. A*, **118**, 7442-7453 (2014).
  141. “A Polymer Brush Based Nanovalve Controlled by Nanoparticle Additives: Design Principles”, R.D. Coalson, A.E. Nasrabad, D. Jasnow, and A Zilman, *J. Phys. Chem. B*, **119**, 11858–11866 (2015).
  142. “Computational Study of Water and Ion Permeability in a Model of Claudin”, R. Laghaei, A.S.L. Yu and R.D. Coalson”, *Proteins (Structure, Function and Bioinformatics)*, **84**, 305–315 (2016).
  - 143 “Simple Biophysics Underpins Collective Conformations of the Intrinsically Disordered Proteins of the Nuclear Pore Complex”, A. Vovk, C. Gu, M.G. Opferman, L. E. Kapinos, R.Y. H. Lim, R.D. Coalson, D. Jasnow, and A. Zilman, *eLife* **5**:e10785:1-29 (2016).
  - 144 “Precise Control of Polymer Coated Nanopores by Nanoparticle Additives: Insights from Computational Modeling”, A.E. Nasrabad, D. Jasnow, A. Zilman and R.D. Coalson, *J. Chem. Phys.* **145**, 064901:1-15 (2016).
  - 145 “Free Energy of Nanoparticle Binding to Multivalent Polymeric Substrates”, C. Gu, A. Zilman, R. D. Coalson, D. Jasnow, *J. Phys. Chem. B* **121**, 6425-6435 (2017).
  - 146 “Effects of Cross-linking on Partitioning of Nanoparticles into a Polymer Brush: Coarse-grained Simulations test Simple Approximate Theories”, M. Ozmaian, D. Jasnow, A.E. Nasrabad, A. Zilman and R.D. Coalson, *J. Chem. Phys.* **148**, 024902:1-12 (2018).
  - 147 “Calculating Tracer Currents through Narrow Ion Channels: Beyond the Independent Particle Model”, R.D. Coalson and D. Jasnow, *Journal of Physics: Condensed Matter* **30**, 294002:1-11 (2018).
  - 148 “Driven Water/Ion Transport through Narrow Nanopores: a Molecular Dynamics Perspective”, R. D. Coalson, *Faraday Discussions* **209**, 249-257 (2018).
  - 149 “Controlling the Surface Properties of Polymer Coated Colloids via Targeted

- Nanoparticles”, M. Ozmaian, B.A. Freitas and R.D. Coalson, *J. Phys. Chem. B*, **123**, 258-265 (2019).
- 150 "The Role of Cohesiveness on the Selective Permeability of Spatial Assemblies of FG Nucleoporins", C. Gu, A. Vovk, R.D. Coalson, and A. Zilman, *Biophysical Journal* **116**, 1204-1215 (2019).
- 151 “Dynamics of Relaxation and Dressing of a Quenched Bose Polaron”, D. Boyanovsky, D. Jasnow, X-L Wu and R.D. Coalson, *Phys. Rev. A* **100**, 043617:1-21 (2019).