# Rigoberto Hernandez

List of Publications by Year
in descending order

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|---|---|---|---|
| 162 papers | 3,660 citations | 145106 33 h-index | 198040 52 g-index |
| 170 all docs | 170 docs citations | 170 times ranked | 2614 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | On the stability of satellites at unstable libration points of sunâ€“planetâ€“moon systems. Communications in Nonlinear Science and Numerical Simulation, 2022, 104, 106053. | 1.7 | 8 |
| 2 | Transition state dynamics of a driven magnetic free layer. Communications in Nonlinear Science and Numerical Simulation, 2022, 105, 106054. | 1.7 | 1 |
| 3 | Mean first-passage times for solvated LiCN isomerization at intermediate to high temperatures. Journal of Chemical Physics, 2022, 156, 034103. | 1.2 | 1 |
| 4 | Electric Potential of Citrate-Capped Gold Nanoparticles Is Affected by Poly(allylamine hydrochloride) and Salt Concentration. ACS Applied Materials & Interfaces, 2022, 14, 12538-12550. | 4.0 | 8 |
| 5 | Molecular Structure of Single-Stranded DNA on the ZnS Surface of Quantum Dots. ACS Nano, 2022, 16, 6666-6675. | 7.3 | 2 |
| 6 | Unconventional aliphatic fluorophores discovered as the luminescence origin in citric acidâ€“urea carbon dots. Nanoscale, 2022, 14, 9516-9525. | 2.8 | 12 |
| 7 | Implementation of Telescoping Boxes in Adaptive Steered Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 4649-4659. | 2.3 | 8 |
| 8 | Adaptive steered molecular dynamics of biomolecules. Molecular Simulation, 2021, 47, 408-419. | 0.9 | 16 |
| 9 | Dynamics and decay rates of a time-dependent two-saddle system. Physical Review E, 2021, 103, 022121. | 0.8 | 4 |
| 10 | Autonomous Computing Materials. ACS Nano, 2021, 15, 3586-3592. | 7.3 | 14 |
| 11 | Energetics and structure of alanine-rich Î±-helices via adaptive steered molecular dynamics. Biophysical Journal, 2021, 120, 2009-2018. | 0.2 | 13 |
| 12 | Engineered nanoparticle network models for autonomous computing. Journal of Chemical Physics, 2021, 154, 214702. | 1.2 | 5 |
| 13 | A Cuban Campesino in Chemistryâ€™s Academic Court. Journal of Physical Chemistry C, 2021, 125, 16371-16377. | 1.5 | 1 |
| 14 | A Cuban Campesino in Chemistryâ€™s Academic Court. Journal of Physical Chemistry B, 2021, 125, 8261-8267. | 1.2 | 1 |
| 15 | The Middle Science: Traversing Scale In Complex Many-Body Systems. ACS Central Science, 2021, 7, 1271-1287. | 5.3 | 16 |
| 16 | A Cuban Campesino in Chemistryâ€™s Academic Court. Journal of Physical Chemistry A, 2021, 125, 6505-6511. | 1.1 | 4 |
| 17 | Controlling reaction dynamics in chemical model systems through external driving. Physica D: Nonlinear Phenomena, 2021, 427, 133013. | 1.3 | 4 |
| 18 | Building blocks for autonomous computing materials: Dimers, trimers, and tetramers. Journal of Chemical Physics, 2021, 155, 154704. | 1.2 | 4 |

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| 19 | Phase space geometry of isolated to condensed chemical reactions. Journal of Chemical Physics, 2021, 155, 210901. | 1.2 | 6 |
| 20 | Dynamics and Bifurcations on the Normally Hyperbolic Invariant Manifold of a Periodically Driven System with Rank-1 Saddle. Regular and Chaotic Dynamics, 2020, 25, 496-507. | 0.3 | 3 |
| 21 | Surface Curvature and Aminated Side-Chain Partitioning Affect Structure of Poly(oxonorbornenes) Attached to Planar Surfaces and Nanoparticles of Gold. Langmuir, 2020, 36, 10412-10420. | 1.6 | 0 |
| 22 | Optimizing bags of artificial neural networks for the prediction of viability from sparse data. Journal of Chemical Physics, 2020, 153, 054112. | 1.2 | 3 |
| 23 | Thermal decay rates of an activated complex in a driven model chemical reaction. Physical Review E, 2020, 102, 062204. | 0.8 | 1 |
| 24 | Influence of external driving on decays in the geometry of the LiCN isomerization. Journal of Chemical Physics, 2020, 153, 084115. | 1.2 | 13 |
| 25 | Neural network approach for the dynamics on the normally hyperbolic invariant manifold of periodically driven systems. Physical Review E, 2020, 101, 022219. | 0.8 | 8 |
| 26 | Solvent softness effects on unimolecular chemical reaction rate constants. Chemical Physics Letters, 2020, 744, 137182. | 1.2 | 3 |
| 27 | Ionic Environment Affects Bacterial Lipopolysaccharide Packing and Function. Langmuir, 2020, 36, 3149-3158. | 1.6 | 9 |
| 28 | The relative stability of trpzip1 and its mutants determined by computation and experiment. RSC Advances, 2020, 10, 6520-6535. | 1.7 | 11 |
| 29 | Solvation Dynamics in the Cybotactic Region of Gas-Expanded Liquids: A Decade Later. Industrial & Engineering Chemistry Research, 2020, 59, 1646-1655. | 1.8 | 0 |
| 30 | Identifying reaction pathways in phase space via asymptotic trajectories. Physical Chemistry Chemical Physics, 2020, 22, 10087-10105. | 1.3 | 6 |
| 31 | Surface Coating Structure and Its Interaction with Cytochrome c in EG<sub>6</sub>-Coated Nanoparticles Varies with Surface Curvature. Langmuir, 2020, 36, 5030-5039. | 1.6 | 10 |
| 32 | Learning from the Machine: Uncovering Sustainable Nanoparticle Design Rules. Journal of Physical Chemistry C, 2020, 124, 13409-13420. | 1.5 | 11 |
| 33 | Removing Barriers. ACS Symposium Series, 2020, , 91-108. | 0.5 | 2 |
| 34 | Defects in Self-Assembled Monolayers on Nanoparticles Prompt Phospholipid Extraction and Bilayer-Curvature-Dependent Deformations. Journal of Physical Chemistry C, 2019, 123, 27951-27958. | 1.5 | 11 |
| 35 | Preferential Binding of Cytochrome c to Anionic Ligand-Coated Gold Nanoparticles: A Complementary Computational and Experimental Approach. ACS Nano, 2019, 13, 6856-6866. | 7.3 | 31 |
| 36 | Invariant Manifolds and Rate Constants in Driven Chemical Reactions. Journal of Physical Chemistry B, 2019, 123, 2070-2086. | 1.2 | 23 |

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| 37 | Solution NMR Analysis of Ligand Environment in Quaternary Ammonium-Terminated Self-Assembled Monolayers on Gold Nanoparticles: The Effect of Surface Curvature and Ligand Structure. Journal of the American Chemical Society, 2019, 141, 4316-4327. | 6.6 | 66 |
| 38 | Phase-space resolved rates in driven multidimensional chemical reactions. Journal of Chemical Physics, 2019, 151, 244108. | 1.2 | 11 |
| 39 | Mutational Analysis of Neuropeptide Y Reveals Unusual Thermal Stability Linked to Higher-Order Self-Association. ACS Omega, 2018, 3, 2141-2154. | 1.6 | 11 |
| 40 | Neural network approach to time-dependent dividing surfaces in classical reaction dynamics. Physical Review E, 2018, 97, 042309. | 0.8 | 15 |
| 41 | Using an environmentally-relevant panel of Gram-negative bacteria to assess the toxicity of polyallylamine hydrochloride-wrapped gold nanoparticles. Environmental Science: Nano, 2018, 5, 279-288. | 2.2 | 32 |
| 42 | National Diversity Equity Workshop 2013: Focus on Gender Identity and Orientation in Chemistry Faculties. ACS Symposium Series, 2018, , 51-77. | 0.5 | 7 |
| 43 | ACS: Your brick-and-mortar and virtual network all in one. C&EN Global Enterprise, 2018, 96, 34-34. | 0.0 | 0 |
| 44 | Density, Structure, and Stability of Citrate<sup>3â€“</sup> and H<sub>2</sub>citrate<sup>â€“</sup> on Bare and Coated Gold Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 28393-28404. | 1.5 | 23 |
| 45 | Modeling soft core-shell colloids using stochastic hard collision dynamics. Chemical Physics Letters, 2018, 708, 233-240. | 1.2 | 6 |
| 46 | Order parameters in the diffusion of rods through two- and three-dimensional fixed scatterers. Physical Review E, 2018, 98, . | 0.8 | 0 |
| 47 | Lipid Corona Formation from Nanoparticle Interactions with Bilayers. CheM, 2018, 4, 2709-2723. | 5.8 | 46 |
| 48 | Binary contraction method for the construction of time-dependent dividing surfaces in driven chemical reactions. Physical Review E, 2018, 98, . | 0.8 | 19 |
| 49 | National Diversity Equity Workshop 2011: Lowering Barriers for all Underrepresented Chemistry Professors. ACS Symposium Series, 2018, , 21-49. | 0.5 | 6 |
| 50 | National Diversity Equity Workshop 2015: Intersectionality in Chemistry Faculties. ACS Symposium Series, 2018, , 79-107. | 0.5 | 7 |
| 51 | National Diversity Equity Workshops: Advancing Diversity in Academia. ACS Symposium Series, 2018, , 1-19. | 0.5 | 6 |
| 52 | Adsorption Dynamics and Structure of Polycations on Citrate-Coated Gold Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 19962-19969. | 1.5 | 21 |
| 53 | Peripheral Membrane Proteins Facilitate Nanoparticle Binding at Lipid Bilayer Interfaces. Langmuir, 2018, 34, 10793-10805. | 1.6 | 24 |
| 54 | National Diversity Equity Workshop 2017: Focus on Underrepresented Minorities in Chemistry Faculties. ACS Symposium Series, 2018, , 109-140. | 0.5 | 8 |

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| 55 | Quantal treatment of O2–Ar vibrational relaxation at hypersonic temperatures. , 2017, , . | | 1 |
| 56 | Leadership Training for Teacher-Scholars. ACS Symposium Series, 2017, , 35-49. | 0.5 | 0 |
| 57 | Accelerating Change: #DiversitySolutions on Social Media. ACS Symposium Series, 2017, , 67-75. | 0.5 | 2 |
| 58 | Obtaining time-dependent multi-dimensional dividing surfaces using Lagrangian descriptors. Chemical Physics Letters, 2017, 687, 194-199. | 1.2 | 33 |
| 59 | Chemical dynamics between wells across a time-dependent barrier: Self-similarity in the Lagrangian descriptor and reactive basins. Journal of Chemical Physics, 2017, 147, 064101. | 1.2 | 29 |
| 60 | Transition state theory for activated systems with driven anharmonic barriers. Journal of Chemical Physics, 2017, 147, 074104. | 1.2 | 19 |
| 61 | OneChemistry in the marketplace of ideas. C&EN Global Enterprise, 2017, 95, 41-41. | 0.0 | 4 |
| 62 | Variational principle for the determination of unstable periodic orbits and instanton trajectories at saddle points. Physical Review A, 2017, 95, . | 1.0 | 4 |
| 63 | The Gender and URM Faculty Demographics Data Collected by OXIDE. ACS Symposium Series, 2017, , 101-112. | 0.5 | 11 |
| 64 | Lagrangian descriptors of driven chemical reaction manifolds. Physical Review E, 2017, 96, 022222. | 0.8 | 35 |
| 65 | Academic leadership skills 101. C&EN Global Enterprise, 2016, 94, 47-47. | 0.0 | 0 |
| 66 | Solvated molecular dynamics of LiCN isomerization: All-atom argon solvent versus a generalized Langevin bath. Journal of Chemical Physics, 2016, 144, 024104. | 1.2 | 15 |
| 67 | Research highlights: examining the effect of shape on nanoparticle interactions with organisms. Environmental Science: Nano, 2016, 3, 696-700. | 2.2 | 13 |
| 68 | Transition state theory for solvated reactions beyond recrossing-free dividing surfaces. Physical Review E, 2016, 93, 062304. | 0.8 | 9 |
| 69 | Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies. Journal of Physical Chemistry B, 2016, 120, 7297-7306. | 1.2 | 52 |
| 70 | Quantum and quasi-classical collisional dynamics of O<sub>2</sub>â€“Ar at high temperatures. Journal of Chemical Physics, 2016, 144, 234311. | 1.2 | 14 |
| 71 | Transition state geometry of driven chemical reactions on time-dependent double-well potentials. Physical Chemistry Chemical Physics, 2016, 18, 30270-30281. | 1.3 | 37 |
| 72 | Lagrangian descriptors in dissipative systems. Physical Chemistry Chemical Physics, 2016, 18, 30282-30287. | 1.3 | 16 |

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| 73 | Uncovering the Geometry of Barrierless Reactions Using Lagrangian Descriptors. Journal of Physical Chemistry B, 2016, 120, 1720-1725. | 1.2 | 35 |
| 74 | Kinetics of intra- and intermolecular excited-state proton transfer ofÏ‰-(2-hydroxynaphthyl-1)-decanoic acid in homogeneous and micellar solutions. Methods and Applications in Fluorescence, 2016, 4, 014001. | 1.1 | 2 |
| 75 | Deconstructing field-induced ketene isomerization through Lagrangian descriptors. Physical Chemistry Chemical Physics, 2016, 18, 4008-4018. | 1.3 | 49 |
| 76 | Determining the Energetics of Small Î²-Sheet Peptides using Adaptive Steered Molecular Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 2028-2037. | 2.3 | 22 |
| 77 | Nonequilibrium structure in sequential assembly. Physical Review E, 2015, 92, 052108. | 0.8 | 2 |
| 78 | Lagrangian Descriptors of Thermalized Transition States on Time-Varying Energy Surfaces. Physical Review Letters, 2015, 115, 148301. | 2.9 | 68 |
| 79 | The Private Sectorâ€™s Role In Chemistryâ€™s Future. Chemical & Engineering News, 2015, 93, 33. | 0.2 | 3 |
| 80 | Diversity In Academia: Solutions To Get There. Chemical & Engineering News, 2015, 93, 40. | 0.2 | 5 |
| 81 | Constrained Unfolding of a Helical Peptide: Implicit versus Explicit Solvents. PLoS ONE, 2015, 10, e0127034. | 1.1 | 33 |
| 82 | Biological Responses to Engineered Nanomaterials: Needs for the Next Decade. ACS Central Science, 2015, 1, 117-123. | 5.3 | 121 |
| 83 | Chemical reactions induced by oscillating external fields in weak thermal environments. Journal of Chemical Physics, 2015, 142, 074108. | 1.2 | 28 |
| 84 | Stochastic dynamics of penetrable rods in one dimension: Entangled dynamics and transport properties. Journal of Chemical Physics, 2015, 142, 154906. | 1.2 | 5 |
| 85 | Multiple branched adaptive steered molecular dynamics. Journal of Chemical Physics, 2014, 141, 064101. | 1.2 | 43 |
| 86 | Dynamical simulation of electrostatic striped colloidal particles. Journal of Chemical Physics, 2014, 140, 034701. | 1.2 | 6 |
| 87 | Persistence of transition-state structure in chemical reactions driven by fields oscillating in time. Physical Review E, 2014, 89, 040801. | 0.8 | 23 |
| 88 | Advancing The Chemical Sciences Through Diversity. Chemical & Engineering News, 2014, 92, 45. | 0.2 | 11 |
| 89 | Communication: Transition state trajectory stability determines barrier crossing rates in chemical reactions induced by time-dependent oscillating fields. Journal of Chemical Physics, 2014, 141, 041106. | 1.2 | 27 |
| 90 | The role of the CN vibration in the activated dynamics of LiNC$ightleftharpoons$â‡ŒLiCN isomerization in an argon solvent at high temperatures. Journal of Chemical Physics, 2014, 141, 074312. | 1.2 | 14 |

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| 91 | Molecular dynamics out of equilibrium: mechanics and measurables. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 541-561. | 6.2 | 11 |
| 92 | Structure of a tractable stochastic mimic of soft particles. Soft Matter, 2014, 10, 5350-5361. | 1.2 | 11 |
| 93 | Effective Surface Coverage of Coarse-Grained Soft Matter. Journal of Physical Chemistry B, 2014, 118, 14092-14102. | 1.2 | 5 |
| 94 | Revisiting roaming trajectories in ketene isomerization at higher dimensionality. Theoretical Chemistry Accounts, 2014, 133, 1. | 0.5 | 8 |
| 95 | A Top-Down Approach for Diversity and Inclusion in Chemistry Departments. ACS Symposium Series, 2014, , 207-224. | 0.5 | 9 |
| 96 | Effects of Roaming Trajectories on the Transition State Theory Rates of a Reduced-Dimensional Model of Ketene Isomerization. Journal of Physical Chemistry A, 2013, 117, 7553-7560. | 1.1 | 24 |
| 97 | Dynamical simulation of dipolar Janus colloids: Dynamical properties. Journal of Chemical Physics, 2013, 138, 184903. | 1.2 | 12 |
| 98 | Stochastic dynamics of penetrable rods in one dimension: Occupied volume and spatial order. Journal of Chemical Physics, 2013, 138, 244901. | 1.2 | 9 |
| 99 | Temperature-driven irreversible generalized Langevin equation can capture the nonequilibrium dynamics of two dissipated coupled oscillators. Physical Review E, 2013, 88, 032145. | 0.8 | 5 |
| 100 | Dynamical simulation of dipolar Janus colloids: Equilibrium structure and thermodynamics. Journal of Chemical Physics, 2012, 137, 044505. | 1.2 | 22 |
| 101 | Adaptive steered molecular dynamics: Validation of the selection criterion and benchmarking energetics in vacuum. Journal of Chemical Physics, 2012, 136, 215104. | 1.2 | 72 |
| 102 | Detailed study of the direct numerical observation of the Kramers turnover in the LiNCâ‡ŒLiCN isomerization rate. Journal of Chemical Physics, 2012, 137, 204301. | 1.2 | 18 |
| 103 | Thermodynamics of Decaalanine Stretching in Water Obtained by Adaptive Steered Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 4837-4844. | 2.3 | 52 |
| 104 | Diffusion of a Spherical Probe through Static Nematogens: Effect of Increasing Geometric Anisotropy and Long-Range Structure. Journal of Physical Chemistry B, 2012, 116, 1328-1334. | 1.2 | 9 |
| 105 | Diffusional effects on the reversible excited-state proton transfer. From experiments to Brownian dynamics simulations. Physical Chemistry Chemical Physics, 2011, 13, 14914. | 1.3 | 34 |
| 106 | Absence of Enhanced Diffusion in the Dynamics of a Thick Needle through Three-Dimensional Fixed Spherical Scatterers. Journal of Physical Chemistry B, 2011, 115, 4412-4418. | 1.2 | 9 |
| 107 | Sifting a Massive Virtual Library of Peptide Ligands for an Optimal Binder to a Given Receptor. Biophysical Journal, 2011, 100, 214a. | 0.2 | 0 |
| 108 | Adaptive Steered Molecular Dynamics: Unfolding of Neuropeptide Y and Decaalanine Stretching. Biophysical Journal, 2011, 100, 524a. | 0.2 | 1 |

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| 109 | Nonequilibrium heat flows through a nanorod sliding across a surface. Journal of Chemical Physics, 2011, 134, 104703. | 1.2 | 5 |
| 110 | Transition state theory in liquids beyond planar dividing surfaces. Chemical Physics, 2010, 370, 270-276. | 0.9 | 68 |
| 111 | Adaptive Steered Molecular Dynamics of the Long-Distance Unfolding of Neuropeptide Y. Journal of Chemical Theory and Computation, 2010, 6, 3026-3038. | 2.3 | 88 |
| 112 | Observation of a Trapping Transition in the Diffusion of a Thick Needle through Fixed Point Scatterers. Journal of Physical Chemistry A, 2010, 114, 9628-9634. | 1.1 | 17 |
| 113 | De novo identification of binding sequences for antibody replacement molecules. Proteins: Structure, Function and Bioinformatics, 2009, 76, 693-705. | 1.5 | 1 |
| 114 | Viewing the Cybotactic Structure of Gas-Expanded Liquids. ACS Symposium Series, 2009, , 81-94. | 0.5 | 0 |
| 115 | Femtosecond-Laser Desorption of H<sub>2</sub> (D<sub>2</sub>) from Ru(0001): Quantum and Classical Approaches. Journal of Physical Chemistry C, 2009, 113, 7790-7801. | 1.5 | 30 |
| 116 | Diffusion in a nonequilibrium binary mixture of hard spheres swelling at different rates. Journal of Chemical Physics, 2009, 131, 024503. | 1.2 | 3 |
| 117 | Molecular Dynamics Simulations of Solvation and Solvent Reorganization Dynamics in CO<sub>2</sub>-Expanded Methanol and Acetone. Journal of Chemical Theory and Computation, 2009, 5, 267-275. | 2.3 | 9 |
| 118 | Momentum and Velocity Autocorrelation Functions of a Diatomic Molecule Are Not Necessarily Proportional to Each Other. Journal of Physical Chemistry B, 2008, 112, 213-218. | 1.2 | 10 |
| 119 | Effects of Solute Structure on Local Solvation and Solvent Interactions: Results from UV/Vis Spectroscopy and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 14993-14998. | 1.2 | 10 |
| 120 | Transition-State Theory Rate Calculations with a Recrossing-Free Moving Dividing Surface. Journal of Physical Chemistry B, 2008, 112, 206-212. | 1.2 | 22 |
| 121 | A Spectroscopic and Computational Exploration of the Cybotactic Region of Gas-Expanded Liquids:â€‰ Methanol and Acetone. Journal of Physical Chemistry B, 2008, 112, 4666-4673. | 1.2 | 23 |
| 122 | Stochastic Models for Polymerization Reactions Under Nonequilibrium Conditions. Annual Reports in Computational Chemistry, 2008, 4, 173-199. | 0.9 | 1 |
| 123 | Solvent-Induced Acceleration of the Rate of Activation of a Molecular Reaction. Physical Review Letters, 2008, 101, 178302. | 2.9 | 40 |
| 124 | Ontology of temperature in nonequilibrium systems. Journal of Chemical Physics, 2007, 126, 244506. | 1.2 | 33 |
| 125 | Chapter 8 The Role of Long-Time Correlation in Dissipative Adsorbate Dynamics on Metal Surfaces. Annual Reports in Computational Chemistry, 2007, 3, 137-151. | 0.9 | 0 |
| 126 | Dihedral-Angle Information Entropy as a Gauge of Secondary Structure Propensity. Biophysical Journal, 2006, 91, 4014-4023. | 0.2 | 4 |

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| 127 | Probing the Cybotactic Region in Gas-Expanded Liquids (GXLs). Accounts of Chemical Research, 2006, 39, 531-538. | 7.6 | 65 |
| 128 | Molecular Dynamics Simulation of the Cybotactic Region in Gas-Expanded Methanolâ"Carbon Dioxide and Acetoneâ"Carbon Dioxide Mixtures. Journal of Physical Chemistry B, 2006, 110, 24101-24111. | 1.2 | 36 |
| 129 | Dynamics of Swelling/Contracting Hard Spheres Surmised by an Irreversible Langevin Equationâ€. Journal of Physical Chemistry A, 2006, 110, 1635-1644. | 1.1 | 19 |
| 130 | Identifying reactive trajectories using a moving transition state. Journal of Chemical Physics, 2006, 124, 244310. | 1.2 | 47 |
| 131 | Dissipating the Langevin equation in the presence of an external stochastic potential. Journal of Chemical Physics, 2005, 122, 114111. | 1.2 | 12 |
| 132 | An idealized model for nonequilibrium dynamics in molecular systems. Journal of Chemical Physics, 2005, 123, 144109. | 1.2 | 14 |
| 133 | Transition State in a Noisy Environment. Physical Review Letters, 2005, 95, 058301. | 2.9 | 75 |
| 134 | Chemical reaction dynamics within anisotropic solvents in time-dependent fields. Journal of Chemical Physics, 2005, 122, 014509. | 1.2 | 21 |
| 135 | Stochastic transition states: Reaction geometry amidst noise. Journal of Chemical Physics, 2005, 123, 204102. | 1.2 | 57 |
| 136 | Folding behavior of model proteins with weak energetic frustration. Journal of Chemical Physics, 2004, 120, 11292-11303. | 1.2 | 11 |
| 137 | A Phenomenological Model for Surface Diffusion:Â Diffusive Dynamics across Incoherent Stochastic Aperiodic Potentials. Journal of Physical Chemistry B, 2004, 108, 19476-19482. | 1.2 | 10 |
| 138 | Mechanism for Radical Cation Transport in Duplex DNA Oligonucleotides. Journal of the American Chemical Society, 2004, 126, 2877-2884. | 6.6 | 84 |
| 139 | On the accuracy limits of orbital expansion methods: Explicit effects ofk-functions on atomic and molecular energies. Journal of Chemical Physics, 2003, 118, 8594-8610. | 1.2 | 70 |
| 140 | An optimized mean first passage time approach for obtaining rates in activated processes. Journal of Chemical Physics, 2002, 117, 9227-9233. | 1.2 | 7 |
| 141 | Activated Dynamics Across Aperiodic Stochastic Potentialsâ€. Journal of Physical Chemistry B, 2002, 106, 8176-8181. | 1.2 | 8 |
| 142 | A three-dimensional polymer growth model. Journal of Chemical Physics, 2002, 116, 10485-10491. | 1.2 | 6 |
| 143 | Important fluctuation dynamics of large protein structures are preserved upon coarse-grained renormalization. International Journal of Quantum Chemistry, 2002, 90, 822-837. | 1.0 | 23 |
| 144 | Nonstationary Stochastic Dynamics and Applications to Chemical Physics. Progress in Theoretical Chemistry and Physics, 2002, , 91-116. | 0.2 | 2 |

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| 145 | Fast Numerical Integrator for Stochastic Differential Equations with Nonstationary Multiplicative Noiseâ€. Journal of Physical Chemistry A, 2001, 105, 2687-2693. | 1.1 | 5 |
| 146 | A minimalist model protein with multiple folding funnels. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 9074-9079. | 3.3 | 18 |
| 147 | Chemical reaction dynamics with stochastic potentials below the high-friction limit. Journal of Chemical Physics, 2001, 115, 2430-2438. | 1.2 | 20 |
| 148 | A two-dimensional polymer growth model. Journal of Chemical Physics, 2001, 115, 1575-1585. | 1.2 | 6 |
| 149 | Stochastic Dynamics in Irreversible Nonequilibrium Environments. 4. Self-Consistent Coupling in Heterogeneous Environments. Journal of Physical Chemistry B, 2000, 104, 3456-3462. | 1.2 | 17 |
| 150 | The projection of a mechanical system onto the irreversible generalized Langevin equation. Journal of Chemical Physics, 1999, 111, 7701-7704. | 1.2 | 39 |
| 151 | Stochastic Dynamics in Irreversible Nonequilibrium Environments. 3. Temperature-Ramped Chemical Kinetics. Journal of Physical Chemistry A, 1999, 103, 11004-11010. | 1.1 | 15 |
| 152 | Stochastic Dynamics in Irreversible Nonequilibrium Environments. 1. The Fluctuationâ^'Dissipation Relation. Journal of Physical Chemistry B, 1999, 103, 1064-1069. | 1.2 | 49 |
| 153 | Stochastic Dynamics in Irreversible Nonequilibrium Environments. 2. A Model for Thermosetting Polymerization. Journal of Physical Chemistry B, 1999, 103, 1070-1077. | 1.2 | 31 |
| 154 | Quantum time correlation functions and classical coherence. Chemical Physics, 1998, 233, 243-255. | 0.9 | 65 |
| 155 | On the Feynman path centroid density as a phase space distribution in quantum statistical mechanics. Journal of Chemical Physics, 1995, 103, 5018-5026. | 1.2 | 17 |
| 156 | A combined use of perturbation theory and diagonalization: Application to bound energy levels and semiclassical rate theory. Journal of Chemical Physics, 1994, 101, 9534-9547. | 1.2 | 56 |
| 157 | Semiclassical transition state theory. A new perspective. Chemical Physics Letters, 1993, 214, 129-136. | 1.2 | 180 |
| 158 | A random matrix/transition state theory for the probability distribution of stateâ€specific unimolecular decay rates: Generalization to include total angular momentum conservation and other dynamical symmetries. Journal of Chemical Physics, 1993, 99, 950-962. | 1.2 | 53 |
| 159 | Cumulative reaction probabilities for H+H2â†'H2+H from a knowledge of the anharmonic force field. Chemical Physics Letters, 1992, 192, 407-416. | 1.2 | 67 |
| 160 | Ab initio calculation of anharmonic constants for a transition state, with application to semiclassical transition state tunneling probabilities. Chemical Physics Letters, 1990, 172, 62-68. | 1.2 | 221 |
| 161 | A transition state theoryâ€based statistical distribution of unimolecular decay rates with application to unimolecular decomposition of formaldehyde. Journal of Chemical Physics, 1990, 93, 5657-5666. | 1.2 | 128 |
| 162 | Limits on the transition to Gaussian orthogonal ensemble behavior: Saturated radiationless transitions between strongly coupled potential surfaces. Physical Review A, 1989, 40, 5935-5949. | 1.0 | 12 |