# Gerhard Stock

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3976868/publications.pdf

Version: 2024-02-01

| | | | |
|---|---|---|---|
| 135 papers | 8,866 citations | 44042 48 h-index | 46771 89 g-index |
| 140 all docs | 140 docs citations | 140 times ranked | 5740 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Semiclassical Description of Nonadiabatic Quantum Dynamics. Physical Review Letters, 1997, 78, 578-581. | 2.9 | 456 |
| 2 | Energy landscape of a small peptide revealed by dihedral angle principal component analysis. Proteins: Structure, Function and Bioinformatics, 2004, 58, 45-52. | 1.5 | 363 |
| 3 | Monomer adds to preformed structured oligomers of Abeta-peptides by a two-stage dock-lock mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 111-116. | 3.3 | 344 |
| 4 | Structure and Dynamics of the Homologous Series of Alanine Peptides:Â A Joint Molecular Dynamics/NMR Study. Journal of the American Chemical Society, 2007, 129, 1179-1189. | 6.6 | 304 |
| 5 | Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578. | 1.6 | 285 |
| 6 | Dihedral angle principal component analysis of molecular dynamics simulations. Journal of Chemical Physics, 2007, 126, 244111. | 1.2 | 279 |
| 7 | Surface-hopping modeling of photoinduced relaxation dynamics on coupled potential-energy surfaces. Journal of Chemical Physics, 1997, 107, 6230-6245. | 1.2 | 239 |
| 8 | Peptide conformational heterogeneity revealed from nonlinear vibrational spectroscopy and molecular-dynamics simulations. Journal of Chemical Physics, 2002, 117, 6833-6840. | 1.2 | 219 |
| 9 | Mapping approach to the semiclassical description of nonadiabatic quantum dynamics. Physical Review A, 1999, 59, 64-79. | 1.0 | 213 |
| 10 | Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218. | 23.0 | 205 |
| 11 | Conformational Dynamics of Trialanine in Water. 2. Comparison of AMBER, CHARMM, GROMOS, and OPLS Force Fields to NMR and Infrared Experiments. Journal of Physical Chemistry B, 2003, 107, 5064-5073. | 1.2 | 199 |
| 12 | Nonperturbative approach to femtosecond spectroscopy: General theory and application to multidimensional nonadiabatic photoisomerization processes. Journal of Chemical Physics, 1995, 103, 3998-4011. | 1.2 | 197 |
| 13 | A PELDOR-Based Nanometer Distance Ruler for Oligonucleotides. Journal of the American Chemical Society, 2004, 126, 5722-5729. | 6.6 | 193 |
| 14 | Energy transport in peptide helices. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 12749-12754. | 3.3 | 179 |
| 15 | Construction of the free energy landscape of biomolecules via dihedral angle principal component analysis. Journal of Chemical Physics, 2008, 128, 245102. | 1.2 | 170 |
| 16 | Semiclassical description of nonadiabatic quantum dynamics: Application to the S1â€“S2 conical intersection in pyrazine. Journal of Chemical Physics, 2000, 112, 10282-10292. | 1.2 | 155 |
| 17 | Quantum-Mechanical Modeling of the Femtosecond Isomerization in Rhodopsin. Journal of Physical Chemistry B, 2000, 104, 1146-1149. | 1.2 | 151 |
| 18 | Principal component analysis of molecular dynamics: On the use of Cartesian vs. internal coordinates. Journal of Chemical Physics, 2014, 141, 014111. | 1.2 | 149 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Base-specific spin-labeling of RNA for structure determination. Nucleic Acids Research, 2007, 35, 3128-3143. | 6.5 | 146 |
| 20 | Ab initio-based exciton model of amide I vibrations in peptides: Definition, conformational dependence, and transferability. Journal of Chemical Physics, 2005, 122, 224904. | 1.2 | 127 |
| 21 | Free energy landscape and folding mechanism of a Î²-hairpin in explicit water: A replica exchange molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2005, 61, 795-808. | 1.5 | 125 |
| 22 | Flow of zero-point energy and exploration of phase space in classical simulations of quantum relaxation dynamics. Journal of Chemical Physics, 1999, 111, 65-76. | 1.2 | 117 |
| 23 | Flow of zero-point energy and exploration of phase space in classical simulations of quantum relaxation dynamics. II. Application to nonadiabatic processes. Journal of Chemical Physics, 1999, 111, 77-88. | 1.2 | 107 |
| 24 | Perspective: Identification of collective variables and metastable states of protein dynamics. Journal of Chemical Physics, 2018, 149, 150901. | 1.2 | 105 |
| 25 | A semiclassical selfâ€consistentâ€field approach to dissipative dynamics: The spinâ€“boson problem. Journal of Chemical Physics, 1995, 103, 1561-1573. | 1.2 | 100 |
| 26 | Energy Transport in Peptide Helices: A Comparison between High- and Low-Energy Excitations. Journal of Physical Chemistry B, 2008, 112, 9091-9099. | 1.2 | 92 |
| 27 | Detection of ultrafast molecular-excited-state dynamics with time- and frequency-resolved pump-probe spectroscopy. Physical Review A, 1992, 45, 3032-3040. | 1.0 | 90 |
| 28 | How Complex Is the Dynamics of Peptide Folding?. Physical Review Letters, 2007, 98, 028102. | 2.9 | 85 |
| 29 | Conformational Dynamics of Trialanine in Water:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 2002, 106, 5294-5301. | 1.2 | 83 |
| 30 | Resonance Raman spectroscopy of theS1andS2states of pyrazine: Experiment and first principles calculation of spectra. Journal of Chemical Physics, 1995, 103, 6851-6860. | 1.2 | 81 |
| 31 | Nonequilibrium molecular-dynamics study of the vibrational energy relaxation of peptides in water. Journal of Chemical Physics, 2003, 119, 11350-11358. | 1.2 | 80 |
| 32 | Quantum-classical Liouville description of multidimensional nonadiabatic molecular dynamics. Journal of Chemical Physics, 2001, 114, 2001-2012. | 1.2 | 79 |
| 33 | Identifying Metastable States of Folding Proteins. Journal of Chemical Theory and Computation, 2012, 8, 3810-3819. | 2.3 | 74 |
| 34 | Contact- and distance-based principal component analysis of protein dynamics. Journal of Chemical Physics, 2015, 143, 244114. | 1.2 | 74 |
| 35 | Molecular dynamics simulation study of the binding of purine bases to the aptamer domain of the guanine sensing riboswitch. Nucleic Acids Research, 2009, 37, 4774-4786. | 6.5 | 72 |
| 36 | Inferring Transition Rates of Networks from Populations in Continuous-Time Markov Processes. Journal of Chemical Theory and Computation, 2015, 11, 5464-5472. | 2.3 | 69 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Robust Density-Based Clustering To Identify Metastable Conformational States of Proteins. Journal of Chemical Theory and Computation, 2016, 12, 2426-2435. | 2.3 | 68 |
| 38 | Consistent treatment of quantum-mechanical and classical degrees of freedom in mixed quantum-classical simulations. Journal of Chemical Physics, 1998, 108, 7516-7526. | 1.2 | 67 |
| 39 | Nonequilibrium molecular dynamics simulation of the energy transport through a peptide helix. Journal of Chemical Physics, 2010, 132, 025102. | 1.2 | 66 |
| 40 | Classical Simulation of Quantum Energy Flow in Biomolecules. Physical Review Letters, 2009, 102, 118301. | 2.9 | 65 |
| 41 | Machine Learning of Biomolecular Reaction Coordinates. Journal of Physical Chemistry Letters, 2018, 9, 2144-2150. | 2.1 | 65 |
| 42 | Time-resolved observation of protein allosteric communication. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6804-E6811. | 3.3 | 63 |
| 43 | A semiclassical selfâ€consistentâ€field approach to dissipative dynamics. II. Internal conversion processes. Journal of Chemical Physics, 1995, 103, 2888-2902. | 1.2 | 60 |
| 44 | Nonequilibrium molecular dynamics simulation of a photoswitchable peptide. Chemical Physics, 2006, 323, 36-44. | 0.9 | 60 |
| 45 | Femtosecond pump-probe spectroscopy of electron-transfer systems: a nonperturbative approach. Chemical Physics, 1997, 217, 275-287. | 0.9 | 56 |
| 46 | NMR and MD studies of the temperature-dependent dynamics of RNA YNMG-tetraloops. Nucleic Acids Research, 2008, 36, 1928-1940. | 6.5 | 56 |
| 47 | Structural Flexibility of a Helical Peptide Regulates Vibrational Energy Transport Properties. Journal of Physical Chemistry B, 2008, 112, 15487-15492. | 1.2 | 53 |
| 48 | Free-Energy Landscape of RNA Hairpins Constructed via Dihedral Angle Principal Component Analysis. Journal of Physical Chemistry B, 2009, 113, 16660-16668. | 1.2 | 53 |
| 49 | Multisecond ligand dissociation dynamics from atomistic simulations. Nature Communications, 2020, 11, 2918. | 5.8 | 52 |
| 50 | Femtosecond secondary emission arising from the nonadiabatic photoisomerization in rhodopsin. Chemical Physics, 2000, 259, 297-312. | 0.9 | 50 |
| 51 | Principal component analysis on a torus: Theory and application to protein dynamics. Journal of Chemical Physics, 2017, 147, 244101. | 1.2 | 50 |
| 52 | Photoinduced Conformational Dynamics of a Photoswitchable Peptide: A Nonequilibrium Molecular Dynamics Simulation Study. Biophysical Journal, 2006, 91, 1224-1234. | 0.2 | 49 |
| 53 | Maximum Caliber: A variational approach applied to two-state dynamics. Journal of Chemical Physics, 2008, 128, 194102. | 1.2 | 49 |
| 54 | Multidimensional Langevin modeling of biomolecular dynamics. Journal of Chemical Physics, 2009, 130, 034106. | 1.2 | 48 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Vibrational energy flow in the villin headpiece subdomain: Master equation simulations. Journal of Chemical Physics, 2015, 142, 075101. | 1.2 | 48 |
| 56 | Scaling Rules for Vibrational Energy Transport in Globular Proteins. Journal of Physical Chemistry Letters, 2016, 7, 25-30. | 2.1 | 48 |
| 57 | Metadynamics Enhanced Markov Modeling of Protein Dynamics. Journal of Physical Chemistry B, 2018, 122, 5508-5514. | 1.2 | 48 |
| 58 | A non-equilibrium approach to allosteric communication. Philosophical Transactions of the Royal Society B: Biological Sciences, 2018, 373, 20170187. | 1.8 | 48 |
| 59 | Molecular Dynamics Simulation of the Structure, Dynamics, and Thermostability of the RNA Hairpins uCACGg and cUUCGg. Journal of Physical Chemistry B, 2008, 112, 134-142. | 1.2 | 47 |
| 60 | Mechanism of a photochemical funnel: a dissipative wave-packet dynamics study. Chemical Physics Letters, 2003, 379, 351-358. | 1.2 | 45 |
| 61 | Structure and energy landscape of a photoswitchable peptide: A replica exchange molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2005, 60, 485-494. | 1.5 | 45 |
| 62 | Real-time observation of ligand-induced allosteric transitions in a PDZ domain. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26031-26039. | 3.3 | 45 |
| 63 | SYNTHESIS OF SPIN-LABELED RNAS FOR LONG RANGE DISTANCE MEASUREMENTS BY PELDOR. Nucleosides, Nucleotides and Nucleic Acids, 2005, 24, 771-775. | 0.4 | 44 |
| 64 | Molecular dynamics simulation of cooling: Heat transfer from a photoexcited peptide to the solvent. Journal of Chemical Physics, 2009, 131, 184503. | 1.2 | 41 |
| 65 | Targeted Molecular Dynamics Calculations of Free Energy Profiles Using a Nonequilibrium Friction Correction. Journal of Chemical Theory and Computation, 2018, 14, 6175-6182. | 2.3 | 41 |
| 66 | Construction of the Free Energy Landscape of Peptide Aggregation from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 1471-1479. | 2.3 | 40 |
| 67 | Ultrafastcis-transphotoswitching: A model study. Journal of Chemical Physics, 2002, 116, 1085-1091. | 1.2 | 39 |
| 68 | What NMR Relaxation Can Tell Us about the Internal Motion of an RNA Hairpin:â€‰ A Molecular Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2006, 2, 1228-1236. | 2.3 | 39 |
| 69 | Hierarchical Folding Free Energy Landscape of HP35 Revealed by Most Probable Path Clustering. Journal of Physical Chemistry B, 2014, 118, 7750-7760. | 1.2 | 39 |
| 70 | Vibrational Conical Intersections as a Mechanism of Ultrafast Vibrational Relaxation. Physical Review Letters, 2012, 109, 173201. | 2.9 | 38 |
| 71 | Energy Flow and Long-Range Correlations in Guanine-Binding Riboswitch: A Nonequilibrium Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 9340-9347. | 1.2 | 36 |
| 72 | Structure and Dynamics of an RNA Tetraloop: A Joint Molecular Dynamics and NMR Study. Structure, 2005, 13, 1255-1267. | 1.6 | 35 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Conformational Dynamics of RNA-Peptide Binding: A Molecular Dynamics Simulation Study. Biophysical Journal, 2006, 90, 391-399. | 0.2 | 35 |
| 74 | Identification and Validation of Reaction Coordinates Describing Protein Functional Motion: Hierarchical Dynamics of T4 Lysozyme. Journal of Chemical Theory and Computation, 2017, 13, 5076-5088. | 2.3 | 35 |
| 75 | Ab initio based building block model of amide I vibrations in peptides. Chemical Physics Letters, 2007, 437, 272-276. | 1.2 | 33 |
| 76 | Photocontrolling Proteinâ€“Peptide Interactions: From Minimal Perturbation to Complete Unbinding. Journal of the American Chemical Society, 2019, 141, 10702-10710. | 6.6 | 33 |
| 77 | Principal component analysis of nonequilibrium molecular dynamics simulations. Journal of Chemical Physics, 2019, 150, 204110. | 1.2 | 31 |
| 78 | Classical description of nonadiabatic photoisomerization processes and their realâ€time detection via femtosecond spectroscopy. Journal of Chemical Physics, 1995, 103, 10015-10029. | 1.2 | 30 |
| 79 | Dynamic treatment of vibrational energy relaxation in a heterogeneous and fluctuating environment. Journal of Chemical Physics, 2008, 129, 134110. | 1.2 | 30 |
| 80 | Hierarchical Biomolecular Dynamics: Picosecond Hydrogen Bonding Regulates Microsecond Conformational Transitions. Journal of Chemical Theory and Computation, 2015, 11, 1330-1336. | 2.3 | 30 |
| 81 | Modeling of decoherence and dissipation in nonadiabatic photoreactions by an effective-scaling nonsecular Redfield algorithm. Chemical Physics, 2005, 310, 33-41. | 0.9 | 29 |
| 82 | Through bonds or contacts? Mapping protein vibrational energy transfer using non-canonical amino acids. Nature Communications, 2021, 12, 3284. | 5.8 | 28 |
| 83 | Efficient calculation of femtosecond time-resolved photoelectron spectra: method and application to the ionization of pyrazine. Physical Chemistry Chemical Physics, 2001, 3, 2331-2336. | 1.3 | 27 |
| 84 | Long-Range Conformational Transition of a Photoswitchable Allosteric Protein: Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 13468-13476. | 1.2 | 26 |
| 85 | Dynamical coring of Markov state models. Journal of Chemical Physics, 2019, 150, 094111. | 1.2 | 26 |
| 86 | Nonadiabatic vibrational dynamics and spectroscopy of peptides: A quantum-classical description. Chemical Physics, 2008, 347, 208-217. | 0.9 | 24 |
| 87 | Hidden Complexity of Protein Free-Energy Landscapes Revealed by Principal Component Analysis by Parts. Journal of Physical Chemistry Letters, 2010, 1, 2769-2773. | 2.1 | 24 |
| 88 | Classical formulation of the spectroscopy of nonadiabatic excitedâ€state dynamics. Journal of Chemical Physics, 1993, 99, 1545-1555. | 1.2 | 23 |
| 89 | Long-Range Conformational Response of a PDZ Domain to Ligand Binding and Release: A Molecular Dynamics Study. Journal of Chemical Theory and Computation, 2016, 12, 870-878. | 2.3 | 23 |
| 90 | Quantum and classical vibrational relaxation dynamics of Nâ€methylacetamide on ab initio potential energy surfaces. International Journal of Quantum Chemistry, 2009, 109, 2047-2057. | 1.0 | 22 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Vibrational conical intersections in the water dimer. Molecular Physics, 2013, 111, 2046-2056. | 0.8 | 22 |
| 92 | A Numerical Procedure to Evaluate Memory Effects in Nonâ€Equilibrium Coarseâ€Grained Models. Advanced Theory and Simulations, 2021, 4, 2000197. | 1.3 | 22 |
| 93 | Hierarchical dynamics in allostery following ATP hydrolysis monitored by single molecule FRET measurements and MD simulations. Chemical Science, 2021, 12, 3350-3359. | 3.7 | 22 |
| 94 | Classical description of ultrafast internal conversion processes. The benzene cation. Chemical Physics Letters, 1994, 224, 131-138. | 1.2 | 21 |
| 95 | Approximate calculation of femtosecond pumpâ€“probe spectra monitoring nonadiabatic excited-state dynamics. Journal of Chemical Physics, 2000, 112, 4910-4922. | 1.2 | 21 |
| 96 | A classical model for time- and frequency-resolved spectroscopy of nonadiabatic excited-state dynamics. Chemical Physics Letters, 1992, 197, 396-404. | 1.2 | 20 |
| 97 | Multidimensional Langevin Modeling of Nonoverdamped Dynamics. Physical Review Letters, 2015, 115, 050602. | 2.9 | 20 |
| 98 | Nonadiabatic vibrational dynamics in the HCO2â¯â‹…H2O complex. Journal of Chemical Physics, 2015, 143, 134308. | 1.2 | 20 |
| 99 | Model studies on femtosecond spectroscopy of multidimensional photoisomerization and internal-conversion dynamics. A nonperturbative approach. Chemical Physics Letters, 1994, 228, 665-671. | 1.2 | 19 |
| 100 | Quasiperiodic orbit analysis of nonadiabaticcisâ€“transphotoisomerization dynamics. Journal of Chemical Physics, 2003, 119, 4204-4215. | 1.2 | 18 |
| 101 | Transient Spectral Features of a cisâ¯trans Photoreaction in the Condensed Phase:â€‰ A Model Study. Journal of Physical Chemistry A, 2004, 108, 6464-6473. | 1.1 | 18 |
| 102 | 2D-IR Spectroscopy of an AHA Labeled Photoswitchable PDZ2 Domain. Journal of Physical Chemistry A, 2017, 121, 9435-9445. | 1.1 | 18 |
| 103 | Azidohomoalanine: A Minimally Invasive, Versatile, and Sensitive Infrared Label in Proteins To Study Ligand Binding. Journal of Physical Chemistry B, 2018, 122, 10118-10125. | 1.2 | 18 |
| 104 | Efficient calculation of time- and frequency-resolved spectra: a mixed non-perturbative/perturbative approach. Chemical Physics Letters, 1998, 296, 137-145. | 1.2 | 16 |
| 105 | Model study on the real-time detection of ultrafast nonadiabatic dynamics associated with the Wulf-Chappuis bands of ozone. Chemical Physics Letters, 1992, 200, 163-172. | 1.2 | 15 |
| 106 | Energy Transport Pathways in Proteins: A Non-equilibrium Molecular Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2019, 15, 5750-5757. | 2.3 | 15 |
| 107 | Master equation model to predict energy transport pathways in proteins. Journal of Chemical Physics, 2020, 152, 045103. | 1.2 | 14 |
| 108 | Real Time Observation of Ultrafast Peptide Conformational Dynamics: Molecular Dynamics Simulation vs Infrared Experiment. Journal of Physical Chemistry B, 2011, 115, 13084-13092. | 1.2 | 13 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | MELD-Path Efficiently Computes Conformational Transitions, Including Multiple and Diverse Paths. Journal of Chemical Theory and Computation, 2018, 14, 2109-2116. | 2.3 | 13 |
| 110 | MSMPathfinder: Identification of Pathways in Markov State Models. Journal of Chemical Theory and Computation, 2020, 16, 7874-7882. | 2.3 | 13 |
| 111 | Periodic Orbit Description of Nonadiabatic Quantum Dynamics. Physical Review Letters, 2001, 87, 140404. | 2.9 | 12 |
| 112 | Quasiclassical and semiclassical wave-packet dynamics in periodic potentials. Journal of Chemical Physics, 2003, 119, 5795-5804. | 1.2 | 12 |
| 113 | Influence of Nitroxide Spin Labels on RNA Structure: A Molecular Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2008, 4, 1781-1787. | 2.3 | 12 |
| 114 | Global Langevin model of multidimensional biomolecular dynamics. Journal of Chemical Physics, 2016, 145, 184114. | 1.2 | 12 |
| 115 | Vibrational energy transport in acetylbenzonitrile described by an ab initio-based quantum tier model. Chemical Physics, 2017, 482, 86-92. | 0.9 | 11 |
| 116 | Nonperturbative generalized master equation for the spin-boson problem. Physical Review E, 1995, 51, 3038-3044. | 0.8 | 10 |
| 117 | Data driven Langevin modeling of biomolecular dynamics. Journal of Chemical Physics, 2013, 138, 204106. | 1.2 | 10 |
| 118 | Photoinduced large amplitude motion as mechanism for pure electronic dephasing and its manifestation in continuousâ€wave and timeâ€resolved spectroscopy. Journal of Chemical Physics, 1994, 101, 246-254. | 1.2 | 9 |
| 119 | Classical phase-space analysis of vibronically coupled systems. Journal of Chemical Physics, 2002, 116, 69. | 1.2 | 9 |
| 120 | Classical Calculation of Transient Absorption Spectra Monitoring Ultrafast Electron Transfer Processes. Journal of Chemical Theory and Computation, 2006, 2, 1605-1617. | 2.3 | 9 |
| 121 | Reply to the comment on â€œEnergy landscape of a small peptide revealed by dihedral angle principal component analysisâ€ Proteins: Structure, Function and Bioinformatics, 2006, 64, 798-799. | 1.5 | 9 |
| 122 | Modeling non-Markovian data using Markov state and Langevin models. Journal of Chemical Physics, 2020, 153, 244112. | 1.2 | 9 |
| 123 | Data-Driven Langevin Modeling of Nonequilibrium Processes. Journal of Physical Chemistry B, 2021, 125, 8125-8136. | 1.2 | 7 |
| 124 | Cooperative Protein Allosteric Transition Mediated by a Fluctuating Transmission Network. Journal of Molecular Biology, 2022, 434, 167679. | 2.0 | 7 |
| 125 | Theoretical Description of Secondary Emission Reflecting Ultrafast Nonadiabatic Isomerizationâ€. Journal of Physical Chemistry A, 2001, 105, 2626-2633. | 1.1 | 6 |
| 126 | Classical description of the dynamics and time-resolved spectroscopy of nonadiabatic cisâ€“trans photoisomerization. Chemical Physics, 2006, 329, 109-117. | 0.9 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Simulation of transient infrared spectra of a photoswitchable peptide. Journal of Chemical Physics, 2011, 135, 225102. | 1.2 | 6 |
| 128 | Communication: Microsecond peptide dynamics from nanosecond trajectories: A Langevin approach. Journal of Chemical Physics, 2014, 141, 241102. | 1.2 | 6 |
| 129 | Mechanisms for allosteric activation of protease DegS by ligand binding and oligomerization as revealed from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1690-1705. | 1.5 | 6 |
| 130 | Molecular Origin of Driving-Dependent Friction in Fluids. Journal of Chemical Theory and Computation, 2022, 18, 2816-2825. | 2.3 | 6 |
| 131 | Periodic-Orbit Analysis of Coherent Electron-Transfer Femtosecond Experiments. Journal of Physical Chemistry A, 2002, 106, 8483-8487. | 1.1 | 5 |
| 132 | Improved Wang-Landau sampling through the use of smoothed potential-energy surfaces. Journal of Chemical Physics, 2006, 124, 154107. | 1.2 | 5 |
| 133 | Quantum modeling of transient infrared spectra reflecting photoinduced electron-transfer dynamics. Journal of Chemical Physics, 2006, 124, 114105. | 1.2 | 4 |
| 134 | EFFECT OF THE ION TREATMENT ON AN RNA HAIRPIN: MOLECULAR DYNAMICS STUDY. Indonesian Journal of Chemistry, 2012, 12, 1-11. | 0.3 | 1 |
| 135 | Cover Image, Volume 84, Issue 11. Proteins: Structure, Function and Bioinformatics, 2016, 84, C1. | 1.5 | 0 |