Rui Sun

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7486308/publications.pdf

Version: 2024-02-01

37 papers	1,010 citations	471509 17 h-index	434195 31 g-index
37 all docs	37 docs citations	37 times ranked	864 citing authors

#	Article	IF	Citations
1	Assessing the Intestinal Permeability of Small Molecule Drugs via Diffusion Motion on a Multidimensional Free Energy Surface. Journal of Chemical Theory and Computation, 2022, 18, 503-515.	5.3	10
2	Biophysical properties of tear film lipid layer II. Polymorphism of FAHFA. Biophysical Journal, 2022, 121, 451-458.	0.5	9
3	Spirovetivane- and Eudesmane-Type Sesquiterpenoids Isolated from the Culture Media of Two Cyanobacterial Strains. Journal of Natural Products, 2022, 85, 415-425.	3.0	2
4	The Potential Energy Profile of the HBr⁺ + HCl Bimolecular Collision. Journal of Physical Chemistry A, 2022, 126, 1465-1474.	2.5	4
5	Interpolating Moving Ridge Regression (IMRR): A machine learning algorithm to predict energy gradients for ab initio molecular dynamics simulations. Chemical Physics, 2022, 557, 111482.	1.9	2
6	Coumarinolignans with Reactive Oxygen Species (ROS) and NF-ÎºB Inhibitory Activities from the Roots of Waltheria indica. Molecules, 2022, 27, 3270.	3.8	3
7	Menthol in electronic cigarettes causes biophysical inhibition of pulmonary surfactant. American Journal of Physiology - Lung Cellular and Molecular Physiology, 2022, 323, L165-L177.	2.9	7
8	A chemical dynamics study of the HClÂ+ HCl+ reaction. International Journal of Mass Spectrometry, 2021, 462, 116515.	1.5	7
9	Molecular Dynamics Study of the Interaction between the N-terminal of Î±-Synuclein and a Lipid Bilayer Mimicking Synaptic Vesicles. Journal of Physical Chemistry B, 2021, 125, 1036-1048.	2.6	9
10	A chemical dynamics study of the reaction of the methylidyne radical (CH, X²Î) with dimethylacetylene (CH₃CCCH₃, X¹A_{1g}). Physical Chemistry Chemical Physics, 2021, 24, 578-593.	2.8	12
11	A chemical dynamics study on the gas-phase formation of triplet and singlet C ₅ H ₂ carbenes. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 30142-30150.	7.1	16
12	Theoretical Study of the Dynamics of the HBr⁺ + CO₂ â†' HOCO⁺ + Br Reaction. Journal of Physical Chemistry A, 2020, 124, 9119-9127.	2.5	10
13	A chemical dynamics study on the gas phase formation of thioformaldehyde (H₂CS) and its thiohydroxycarbene isomer (HCSH). Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 22712-22719.	7.1	18
14	6-Deoxy- and 11-Hydroxytolypodiols: Meroterpenoids from the Cyanobacterium HT-58-2. Journal of Natural Products, 2020, 83, 1691-1695.	3.0	8
15	Mycolactone Toxin Membrane Permeation: Atomistic versus Coarse-Grained MARTINI Simulations. Biophysical Journal, 2019, 117, 87-98.	0.5	19
16	Theoretical Study of the Potential Energy Profile of the HBr⁺ + CO₂ â†' HOCO⁺ + BrÂ· Reaction. Journal of Physical Chemistry A, 2019, 123, 9791-9799.	2.5	4
17	Characterization of Leptazolines Aâ€“D, Polar Oxazolines from the Cyanobacterium Leptolyngbya sp., Reveals a Glitch with the â€œWilloughbyâ€“Hoyeâ€•Scripts for Calculating NMR Chemical Shifts. Organic Letters, 2019, 21, 8449-8453.	4.6	45
18	Molecular transport through membranes: Accurate permeability coefficients from multidimensional potentials of mean force and local diffusion constants. Journal of Chemical Physics, 2018, 149, 072310.	3.0	43

#	Article	IF	Citations
19	Simulating Protein Mediated Hydrolysis of ATP and Other Nucleoside Triphosphates by Combining QM/MM Molecular Dynamics with Advances in Metadynamics. Journal of Chemical Theory and Computation, 2017, 13, 2332-2341.	5.3	40
20	Indirect dynamics in S_N2@N: insight into the influence of central atoms. Physical Chemistry Chemical Physics, 2017, 19, 22691-22699.	2.8	12
21	Transition-Tempered Metadynamics Is a Promising Tool for Studying the Permeation of Drug-like Molecules through Membranes. Journal of Chemical Theory and Computation, 2016, 12, 5157-5169.	5.3	54
22	Comparison of direct dynamics simulations with different electronic structure methods. F^{â˜} + CH₃I with MP2 and DFT/B97-1. Physical Chemistry Chemical Physics, 2015, 17, 2589-2597.	2.8	47
23	Potential energy surfaces for the HBr+ + CO2 â†' Br + HOCO+ reaction in the HBr+â€‰2Î3/2 and 2Î1/2 spin-orbit states. Journal of Chemical Physics, 2015, 142, 104302.	3.0	6
24	Exploring Valleys without Climbing Every Peak: More Efficient and Forgiving Metabasin Metadynamics via Robust On-the-Fly Bias Domain Restriction. Journal of Chemical Theory and Computation, 2015, 11, 5638-5650.	5.3	31
25	The Fâ˜+ CH3I â†' FCH3+ Iâ˜ entrance channel potential energy surface. International Journal of Mass Spectrometry, 2015, 377, 222-227.	1.5	19
26	A unified model for simulating liquid and gas phase, intermolecular energy transfer: N2 + C6F6 collisions. Journal of Chemical Physics, 2014, 140, 194103.	3.0	30
27	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. Computer Physics Communications, 2014, 185, 1074-1080.	7.5	93
28	Direct Dynamics Simulation of the Activation and Dissociation of 1,5-Dinitrobiuret (HDNB). Journal of Physical Chemistry A, 2014, 118, 2228-2236.	2.5	12
29	Models for Intrinsic Non-RRKM Dynamics. Decomposition of the SN2 Intermediate Clâ€“â€“CH3Br. Zeitschrift Fur Physikalische Chemie, 2013, 227, .	2.8	8
30	Comparison of Cluster, Slab, and Analytic Potential Models for the Dimethyl Methylphosphonate (DMMP)/TiO₂(110) Intermolecular Interaction. Journal of Physical Chemistry C, 2013, 117, 17613-17622.	3.1	18
31	Direct Dynamics Simulations of the Product Channels and Atomistic Mechanisms for the OH^{â€“} + CH₃I Reaction. Comparison with Experiment. Journal of Physical Chemistry A, 2013, 117, 7162-7178.	2.5	73
32	Direct chemical dynamics simulations: coupling of classical and quasiclassical trajectories with electronic structure theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 296-316.	14.6	93
33	Indirect Dynamics in a Highly Exoergic Substitution Reaction. Journal of the American Chemical Society, 2013, 135, 4250-4259.	13.7	94
34	Simulation studies of the Clâ˜ + CH3I SN2 nucleophilic substitution reaction: Comparison with ion imaging experiments. Journal of Chemical Physics, 2013, 138, 114309.	3.0	55
35	Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. Journal of Chemical Theory and Computation, 2012, 8, 1212-1222.	5.3	46
36	Direct dynamics simulation of dioxetane formation and decomposition via the singlet Â·Oâ€“Oâ€“CH2â€“CH2Â· biradical: Non-RRKM dynamics. Journal of Chemical Physics, 2012, 137, 044305.	3.0	22

#	Article	IF	Citations
37	Use of Direct Dynamics Simulations to Determine Unimolecular Reaction Paths and Arrhenius Parameters for Large Molecules. Journal of Chemical Theory and Computation, 2011, 7, 3478-3483.	5.3	29