Rui Sun

List of Publications by Year
in descending order

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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	Indirect Dynamics in a Highly Exoergic Substitution Reaction. Journal of the American Chemical Society, 2013, 135, 4250-4259.	13.7	94
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	The Fâ^'+ CH3I â†' FCH3+ Iâ^' entrance channel potential energy surface. International Journal of Mass Spectrometry, 2015, 377, 222-227.	1.5	19
17	Mycolactone Toxin Membrane Permeation: Atomistic versus Coarse-Grained MARTINI Simulations. Biophysical Journal, 2019, 117, 87-98.	0.5	19
18	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

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19	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
20	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
21	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
22	Indirect dynamics in S_N2@N: insight into the influence of central atoms. Physical Chemistry Chemical Physics, 2017, 19, 22691-22699.	2.8	12
23	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
24	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
25	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
26	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
27	Biophysical properties of tear film lipid layer II. Polymorphism of FAHFA. Biophysical Journal, 2022, 121, 451-458.	0.5	9
28	Models for Intrinsic Non-RRKM Dynamics. Decomposition of the SN2 Intermediate Clâ€"â€"CH3Br. Zeitschrift Fur Physikalische Chemie, 2013, 227, .	2.8	8
29	6-Deoxy- and 11-Hydroxytolypodiols: Meroterpenoids from the Cyanobacterium HT-58-2. Journal of Natural Products, 2020, 83, 1691-1695.	3.0	8
30	A chemical dynamics study of the HClÂ+ HCl+ reaction. International Journal of Mass Spectrometry, 2021, 462, 116515.	1.5	7
31	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
32	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
33	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
34	The Potential Energy Profile of the HBr⁺ + HCl Bimolecular Collision. Journal of Physical Chemistry A, 2022, 126, 1465-1474.	2.5	4
35	Coumarinolignans with Reactive Oxygen Species (ROS) and NF-ÎºB Inhibitory Activities from the Roots of Waltheria indica. Molecules, 2022, 27, 3270.	3.8	3
36	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

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37	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