Max Buchholz

List of Publications by Year
in descending order

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45	1,498	218677	315739
papers	citations	26 h-index	38 g-index

46	46	46	497
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Zwitter Ionization of Glycine at Outer Space Conditions due to Microhydration by Six Water Molecules. Physical Review Letters, 2022, 128, 033001.	7.8	7
2	Quantum Vibrational Spectroscopy of Explicitly Solvated Thymidine in Semiclassical Approximation. Journal of Physical Chemistry Letters, 2022, 13, 1350-1355.	4.6	8
3	How many water molecules are needed to solvate one?. Chemical Science, 2021, 12, 2060-2064.	7.4	44
4	Caldeiraâ€“Leggett model vs ab initio potential: A vibrational spectroscopy test of water solvation. Journal of Chemical Physics, 2021, 154, 094106.	3.0	18
5	Unsupervised Machine Learning Neural Gas Algorithm for Accurate Evaluations of the Hessian Matrix in Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 6733-6746.	5.3	7
6	On-the-fly adiabatically switched semiclassical initial value representation molecular dynamics for vibrational spectroscopy of biomolecules. Journal of Chemical Physics, 2021, 155, 234102.	3.0	13
7	Sensitivity of semiclassical vibrational spectroscopy to potential energy surface accuracy: A test on formaldehyde. Vibrational Spectroscopy, 2020, 106, 103015.	2.2	6
8	Anharmonic quantum nuclear densities from full dimensional vibrational eigenfunctions with application to protonated glycine. Nature Communications, 2020, 11, 4348.	12.8	24
9	Semiclassical Vibrational Spectroscopy of Biological Molecules Using Force Fields. Journal of Chemical Theory and Computation, 2020, 16, 3476-3485.	5.3	18
10	Anharmonic calculations of vibrational spectra for molecular adsorbates: A divide-and-conquer semiclassical molecular dynamics approach. Journal of Chemical Physics, 2020, 152, 104104.	3.0	18
11	Representing molecular ground and excited vibrational eigenstates with nuclear densities obtained from semiclassical initial value representation molecular dynamics. Journal of Chemical Physics, 2020, 153, 214117.	3.0	13
12	Machine learning for vibrational spectroscopy via divide-and-conquer semiclassical initial value representation molecular dynamics with application to N-methylacetamide. Journal of Chemical Physics, 2020, 153, 204104.	3.0	23
13	Semiclassical vibrational spectroscopy with Hessian databases. Journal of Chemical Physics, 2019, 150, 244118.	3.0	25
14	Vibrational investigation of nucleobases by means of divide and conquer semiclassical dynamics. Journal of Chemical Physics, 2019, 150, 224107.	3.0	29
15	An effective semiclassical approach to IR spectroscopy. Journal of Chemical Physics, 2019, 150, 184113.	3.0	29
16	Improved semiclassical dynamics through adiabatic switching trajectory sampling. Journal of Chemical Physics, 2019, 151, 214107.	3.0	24
17	Simplified approach to the mixed time-averaging semiclassical initial value representation for the calculation of dense vibrational spectra. Journal of Chemical Physics, 2018, 148, 114107.	3.0	32
18	â€œDivide and conquerâ€•semiclassical molecular dynamics: A practical method for spectroscopic calculations of high dimensional molecular systems. Journal of Chemical Physics, 2018, 148, 014307.	3.0	39

#	Article	IF	Citations
19	â€œDivide-and-conquerâ€•semiclassical molecular dynamics: An application to water clusters. Journal of Chemical Physics, 2018, 148, 104302.	3.0	38
20	A quantum mechanical insight into SN2 reactions: Semiclassical initial value representation calculations of vibrational features of the Clâ¯â‹¯CH3Cl pre-reaction complex with the VENUS suite of codes. Journal of Chemical Physics, 2018, 149, 164113.	3.0	19
21	Protonated glycine supramolecular systems: the need for quantum dynamics. Chemical Science, 2018, 9, 7894-7901.	7.4	35
22	Anharmonic vibrational eigenfunctions and infrared spectra from semiclassical molecular dynamics. Journal of Chemical Physics, 2018, 149, 064115.	3.0	28
23	Herman-Kluk propagator is free from zero-point energy leakage. Chemical Physics, 2018, 515, 231-235.	1.9	27
24	On-the-Fly ab Initio Semiclassical Calculation of Glycine Vibrational Spectrum. Journal of Chemical Theory and Computation, 2017, 13, 2378-2388.	5.3	53
25	A quantum method for thermal rate constant calculations from stationary phase approximation of the thermal flux-flux correlation function integral. Journal of Chemical Physics, 2017, 146, 214115.	3.0	10
26	Semiclassical â€œDivide-and-Conquerâ€•Method for Spectroscopic Calculations of High Dimensional Molecular Systems. Physical Review Letters, 2017, 119, 010401.	7.8	57
27	Application of the mixed time-averaging semiclassical initial value representation method to complex molecular spectra. Journal of Chemical Physics, 2017, 147, 164110.	3.0	30
28	The importance of the pre-exponential factor in semiclassical molecular dynamics. Journal of Chemical Physics, 2016, 145, 144107.	3.0	36
29	Mixed semiclassical initial value representation time-averaging propagator for spectroscopic calculations. Journal of Chemical Physics, 2016, 144, 094102.	3.0	40
30	An Efficient Computational Approach for the Calculation of the Vibrational Density of States. Journal of Physical Chemistry A, 2016, 120, 4853-4862.	2.5	18
31	Graphics processing units accelerated semiclassical initial value representation molecular dynamics. Journal of Chemical Physics, 2014, 140, 174109.	3.0	30
32	Helium Isotope Enrichment by Resonant Tunneling through Nanoporous Graphene Bilayers. Journal of Physical Chemistry A, 2014, 118, 6457-6465.	2.5	27
33	Reproducing Deep Tunneling Splittings, Resonances, and Quantum Frequencies in Vibrational Spectra From a Handful of Direct Ab Initio Semiclassical Trajectories. Journal of Physical Chemistry Letters, 2013, 4, 3407-3412.	4.6	45
34	Deep nuclear resonant tunneling thermal rate constant calculations. International Journal of Quantum Chemistry, 2013, 113, 1722-1734.	2.0	9
35	Evaluating the Accuracy of Hessian Approximations for Direct Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 54-64.	5.3	44
36	Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme. Journal of Chemical Physics, 2013, 138, 054116.	3.0	50

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37	Semiclassical Hybrid Approach to Condensed Phase Molecular Dynamics: Application to the I₂Kr₁₇ Cluster. Journal of Physical Chemistry A, 2012, 116, 11199-11210.	2.5	19
38	First principles semiclassical calculations of vibrational eigenfunctions. Journal of Chemical Physics, 2011, 134, 234103.	3.0	35
39	Fighting the curse of dimensionality in first-principles semiclassical calculations: Non-local reference states for large number of dimensions. Journal of Chemical Physics, 2011, 135, 214108.	3.0	45
40	Multiple coherent states semiclassical initial value representation spectra calculations of lateral interactions for CO on Cu(100). Journal of Chemical Physics, 2010, 133, 054701.	3.0	35
41	Multiple coherent states for first-principles semiclassical initial value representation molecular dynamics. Journal of Chemical Physics, 2009, 130, 234113.	3.0	82
42	First-principles semiclassical initial value representation molecular dynamics. Physical Chemistry Chemical Physics, 2009, 11, 3861.	2.8	70
43	Quantum reaction rate from higher derivatives of the thermal flux-flux autocorrelation function at time zero. Journal of Chemical Physics, 2005, 122, 044109.	3.0	30
44	Test of the quantum instanton approximation for thermal rate constants for some collinear reactions. Journal of Chemical Physics, 2004, 120, 6356-6362.	3.0	35
45	Quantum instanton approximation for thermal rate constants of chemical reactions. Journal of Chemical Physics, 2003, 119, 1329-1342.	3.0	160