

Alexei A Kananenka

List of Publications by Year in descending order

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Version: 2024-02-01

17
papers

610
citations

623734

14
h-index

888059

17
g-index

17
all docs

17
docs citations

17
times ranked

647
citing authors

#	ARTICLE	IF	CITATIONS
1	Systematically improvable multiscale solver for correlated electron systems. <i>Physical Review B</i> , 2015, 91, .	3.2	77
2	Communication: Towards <i>ab initio</i> self-energy embedding theory in quantum chemistry. <i>Journal of Chemical Physics</i> , 2015, 143, 241102.	3.0	76
3	Fermi resonance in OH-stretch vibrational spectroscopy of liquid water and the water hexamer. <i>Journal of Chemical Physics</i> , 2018, 148, 244107.	3.0	64
4	Accurate Long-Time Mixed Quantum-Classical Liouville Dynamics via the Transfer Tensor Method. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4809-4814.	4.6	49
5	Machine Learning for Vibrational Spectroscopic Maps. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6850-6858.	5.3	49
6	Rigorous Ab Initio Quantum Embedding for Quantum Chemistry Using Green's Function Theory: Screened Interaction, Nonlocal Self-Energy Relaxation, Orbital Basis, and Chemical Accuracy. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4856-4870.	5.3	44
7	Efficient Temperature-Dependent Green's Functions Methods for Realistic Systems: Compact Grids for Orthogonal Polynomial Transforms. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 564-571.	5.3	40
8	Fractional charge and spin errors in self-consistent Green's function theory. <i>Journal of Chemical Physics</i> , 2015, 142, 194108.	3.0	37
9	Nonadiabatic Dynamics via the Symmetrical Quasi-Classical Method in the Presence of Anharmonicity. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 319-326.	4.6	32
10	Efficient Temperature-Dependent Green's Function Methods for Realistic Systems: Using Cubic Spline Interpolation to Approximate Matsubara Green's Functions. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2250-2259.	5.3	30
11	Convolutional Neural Networks for Long Time Dissipative Quantum Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2476-2483.	4.6	28
12	Unusually strong hydrogen bond cooperativity in particular (H ₂ O) ₂₀ clusters. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18124-18131.	2.8	24
13	A comparative study of different methods for calculating electronic transition rates. <i>Journal of Chemical Physics</i> , 2018, 148, 102304.	3.0	18
14	IR Spectroscopy Can Reveal the Mechanism of K ⁺ Transport in Ion Channels. <i>Biophysical Journal</i> , 2020, 118, 254-261.	0.5	17
15	Combining Density Functional Theory and Green's Function Theory: Range-Separated, Nonlocal, Dynamic, and Orbital-Dependent Hybrid Functional. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5317-5331.	5.3	10
16	OH-Stretch Raman Multivariate Curve Resolution Spectroscopy of HOD/H ₂ O Mixtures. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5139-5146.	2.6	10
17	Dephasing and Decoherence in Vibrational and Electronic Line Shapes. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1531-1542.	2.6	5