Alexei A Kananenka

List of Publications by Year
in descending order

17	610	623734 14	888059 17
papers	citations	h-index	g-index

17	17	17	647
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Convolutional Neural Networks for Long Time Dissipative Quantum Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 2476-2483.	4.6	28
2	IR Spectroscopy Can Reveal the Mechanism of K+ Transport in Ion Channels. Biophysical Journal, 2020, 118, 254-261.	0.5	17
3	Unusually strong hydrogen bond cooperativity in particular (H₂O)₂₀clusters. Physical Chemistry Chemical Physics, 2020, 22, 18124-18131.	2.8	24
4	Dephasing and Decoherence in Vibrational and Electronic Line Shapes. Journal of Physical Chemistry B, 2020, 124, 1531-1542.	2.6	5
5	Machine Learning for Vibrational Spectroscopic Maps. Journal of Chemical Theory and Computation, 2019, 15, 6850-6858.	5.3	49
6	OH-Stretch Raman Multivariate Curve Resolution Spectroscopy of HOD/H2O Mixtures. Journal of Physical Chemistry B, 2019, 123, 5139-5146.	2.6	10
7	Nonadiabatic Dynamics via the Symmetrical Quasi-Classical Method in the Presence of Anharmonicity. Journal of Physical Chemistry Letters, 2018, 9, 319-326.	4.6	32
8	A comparative study of different methods for calculating electronic transition rates. Journal of Chemical Physics, 2018, 148, 102304.	3.0	18
9	Fermi resonance in OH-stretch vibrational spectroscopy of liquid water and the water hexamer. Journal of Chemical Physics, 2018, 148, 244107.	3.0	64
10	Combining Density Functional Theory and Greenâ€™s Function Theory: Range-Separated, Nonlocal, Dynamic, and Orbital-Dependent Hybrid Functional. Journal of Chemical Theory and Computation, 2017, 13, 5317-5331.	5.3	10
11	Rigorous Ab Initio Quantum Embedding for Quantum Chemistry Using Greenâ€™s Function Theory: Screened Interaction, Nonlocal Self-Energy Relaxation, Orbital Basis, and Chemical Accuracy. Journal of Chemical Theory and Computation, 2016, 12, 4856-4870.	5.3	44
12	Accurate Long-Time Mixed Quantum-Classical Liouville Dynamics via the Transfer Tensor Method. Journal of Physical Chemistry Letters, 2016, 7, 4809-4814.	4.6	49
13	Efficient Temperature-Dependent Greenâ€™s Function Methods for Realistic Systems: Using Cubic Spline Interpolation to Approximate Matsubara Greenâ€™s Functions. Journal of Chemical Theory and Computation, 2016, 12, 2250-2259.	5.3	30
14	Efficient Temperature-Dependent Greenâ€™s Functions Methods for Realistic Systems: Compact Grids for Orthogonal Polynomial Transforms. Journal of Chemical Theory and Computation, 2016, 12, 564-571.	5.3	40
15	Systematically improvable multiscale solver for correlated electron systems. Physical Review B, 2015, 91, .	3.2	77
16	Communication: Towards ab initio self-energy embedding theory in quantum chemistry. Journal of Chemical Physics, 2015, 143, 241102.	3.0	76
17	Fractional charge and spin errors in self-consistent Greenâ€™s function theory. Journal of Chemical Physics, 2015, 142, 194108.	3.0	37