Liang Shi

List of Publications by Year
in descending order

25	437	623188 14	713013 21
papers	citations	h-index	g-index

26	26	26	600
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Simulating Energy Transfer in Molecular Systems with Digital Quantum Computers. Journal of Chemical Theory and Computation, 2022, 18, 1347-1358.	2.3	4
2	Variational Quantum Simulation of Chemical Dynamics with Quantum Computers. Journal of Chemical Theory and Computation, 2022, 18, 2105-2113.	2.3	7
3	Comparison of Linear Response Theory, Projected Initial Maximum Overlap Method, and Molecular Dynamics-Based Vibronic Spectra: The Case of Methylene Blue. Journal of Chemical Theory and Computation, 2022, 18, 3039-3051.	2.3	2
4	Epitope alteration by small molecules and applications in drug discovery. Chemical Science, 2022, 13, 8104-8116.	3.7	6
5	Vibronic and Environmental Effects in Simulations of Optical Spectroscopy. Annual Review of Physical Chemistry, 2021, 72, 165-188.	4.8	33
6	Î²-Amyloid Peptides Manipulate Switching Behaviors of Donorâ€“Acceptor Stenhouse Adducts. Analytical Chemistry, 2021, 93, 9887-9896.	3.2	4
7	Transfer learning with graph neural networks for optoelectronic properties of conjugated oligomers. Journal of Chemical Physics, 2021, 154, 024906.	1.2	28
8	Determining Partial Atomic Charges for Liquid Water: Assessing Electronic Structure and Charge Models. Journal of Chemical Theory and Computation, 2021, 17, 889-901.	2.3	15
9	Simulation of Condensed-Phase Spectroscopy with Near-Term Digital Quantum Computers. Journal of Chemical Theory and Computation, 2021, 17, 7178-7186.	2.3	8
10	The Influence of Electronic Polarization on Nonlinear Optical Spectroscopy. Journal of Physical Chemistry B, 2021, 125, 12214-12227.	1.2	8
11	Influence of Electronic Polarization on the Spectral Density. Journal of Physical Chemistry B, 2020, 124, 531-543.	1.2	16
12	Nonlinear spectroscopy in the condensed phase: The role of Duschinsky rotations and third order cumulant contributions. Journal of Chemical Physics, 2020, 153, 044127.	1.2	22
13	Machine learning Frenkel Hamiltonian parameters to accelerate simulations of exciton dynamics. Journal of Chemical Physics, 2020, 153, 074111.	1.2	20
14	Deep Learning for Optoelectronic Properties of Organic Semiconductors. Journal of Physical Chemistry C, 2020, 124, 7048-7060.	1.5	35
15	Terahertz-Driven Stark Spectroscopy of CdSe and CdSeâ€“CdS Coreâ€“Shell Quantum Dots. Nano Letters, 2019, 19, 8125-8131.	4.5	15
16	Vibrational solvatochromism of the ester carbonyl vibration of PCBM in organic solutions. Journal of Chemical Physics, 2019, 151, 064501.	1.2	3
17	Mid-IR spectroscopy of supercritical water: From dilute gas to dense fluid. Journal of Chemical Physics, 2019, 150, 054505.	1.2	11
18	Modeling the Influence of Correlated Molecular Disorder on the Dynamics of Excitons in Organic Molecular Semiconductors. Journal of Physical Chemistry C, 2019, 123, 306-314.	1.5	11

#	Article	IF	Citations
19	Percolation in supercritical water: Do the Widom and percolation lines coincide?. Journal of Chemical Physics, 2018, 149, 084504.	1.2	23
20	Modeling the effects of molecular disorder on the properties of Frenkel excitons in organic molecular semiconductors. Journal of Chemical Physics, 2018, 149, 094110.	1.2	14
21	The Enhancement of Interfacial Exciton Dissociation by Energetic Disorder Is a Nonequilibrium Effect. ACS Central Science, 2017, 3, 1262-1270.	5.3	44
22	A Model of Charge-Transfer Excitons: Diffusion, Spin Dynamics, and Magnetic Field Effects. Journal of Physical Chemistry Letters, 2016, 7, 2246-2251.	2.1	18
23	Two-dimensional infrared spectroscopy of neat ice I_h. Physical Chemistry Chemical Physics, 2016, 18, 3772-3779.	1.3	26
24	Heavy snow: IR spectroscopy of isotope mixed crystalline water ice. Physical Chemistry Chemical Physics, 2016, 18, 4978-4993.	1.3	20
25	Reparametrized E3B (Explicit Three-Body) Water Model Using the TIP4P/2005 Model as a Reference. Journal of Chemical Theory and Computation, 2015, 11, 2268-2277.	2.3	43