Liang Shi

List of Publications by Year
in descending order

25 papers	437 citations	623734 14 h-index	713466 21 g-index
26 all docs	26 docs citations	26 times ranked	600 citing authors

#	ARTICLE	IF	CITATIONS
1	The Enhancement of Interfacial Exciton Dissociation by Energetic Disorder Is a Nonequilibrium Effect. ACS Central Science, 2017, 3, 1262-1270.	11.3	44
2	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.	5.3	43
3	Deep Learning for Optoelectronic Properties of Organic Semiconductors. Journal of Physical Chemistry C, 2020, 124, 7048-7060.	3.1	35
4	Vibronic and Environmental Effects in Simulations of Optical Spectroscopy. Annual Review of Physical Chemistry, 2021, 72, 165-188.	10.8	33
5	Transfer learning with graph neural networks for optoelectronic properties of conjugated oligomers. Journal of Chemical Physics, 2021, 154, 024906.	3.0	28
6	Two-dimensional infrared spectroscopy of neat ice I_h. Physical Chemistry Chemical Physics, 2016, 18, 3772-3779.	2.8	26
7	Percolation in supercritical water: Do the Widom and percolation lines coincide?. Journal of Chemical Physics, 2018, 149, 084504.	3.0	23
8	Nonlinear spectroscopy in the condensed phase: The role of Duschinsky rotations and third order cumulant contributions. Journal of Chemical Physics, 2020, 153, 044127.	3.0	22
9	Heavy snow: IR spectroscopy of isotope mixed crystalline water ice. Physical Chemistry Chemical Physics, 2016, 18, 4978-4993.	2.8	20
10	Machine learning Frenkel Hamiltonian parameters to accelerate simulations of exciton dynamics. Journal of Chemical Physics, 2020, 153, 074111.	3.0	20
11	A Model of Charge-Transfer Excitons: Diffusion, Spin Dynamics, and Magnetic Field Effects. Journal of Physical Chemistry Letters, 2016, 7, 2246-2251.	4.6	18
12	Influence of Electronic Polarization on the Spectral Density. Journal of Physical Chemistry B, 2020, 124, 531-543.	2.6	16
13	Terahertz-Driven Stark Spectroscopy of CdSe and CdSe–CdS Core–Shell Quantum Dots. Nano Letters, 2019, 19, 8125-8131.	9.1	15
14	Determining Partial Atomic Charges for Liquid Water: Assessing Electronic Structure and Charge Models. Journal of Chemical Theory and Computation, 2021, 17, 889-901.	5.3	15
15	Modeling the effects of molecular disorder on the properties of Frenkel excitons in organic molecular semiconductors. Journal of Chemical Physics, 2018, 149, 094110.	3.0	14
16	Mid-IR spectroscopy of supercritical water: From dilute gas to dense fluid. Journal of Chemical Physics, 2019, 150, 054505.	3.0	11
17	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.	3.1	11
18	Simulation of Condensed-Phase Spectroscopy with Near-Term Digital Quantum Computers. Journal of Chemical Theory and Computation, 2021, 17, 7178-7186.	5.3	8

#	ARTICLE	IF	CITATIONS
19	The Influence of Electronic Polarization on Nonlinear Optical Spectroscopy. Journal of Physical Chemistry B, 2021, 125, 12214-12227.	2.6	8
20	Variational Quantum Simulation of Chemical Dynamics with Quantum Computers. Journal of Chemical Theory and Computation, 2022, 18, 2105-2113.	5.3	7
21	Epitope alteration by small molecules and applications in drug discovery. Chemical Science, 2022, 13, 8104-8116.	7.4	6
22	β-Amyloid Peptides Manipulate Switching Behaviors of Donor–Acceptor Stenhouse Adducts. Analytical Chemistry, 2021, 93, 9887-9896.	6.5	4
23	Simulating Energy Transfer in Molecular Systems with Digital Quantum Computers. Journal of Chemical Theory and Computation, 2022, 18, 1347-1358.	5.3	4
24	Vibrational solvatochromism of the ester carbonyl vibration of PCBM in organic solutions. Journal of Chemical Physics, 2019, 151, 064501.	3.0	3
25	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.	5.3	2