

Sean A Fischer

List of Publications by Year in descending order

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Version: 2024-02-01

25
papers

1,485
citations

430874

18
h-index

610901

24
g-index

26
all docs

26
docs citations

26
times ranked

1883
citing authors

#	ARTICLE	IF	CITATIONS
1	Decoherence-induced surface hopping. <i>Journal of Chemical Physics</i> , 2012, 137, 22A545.	3.0	491
2	Ice-nucleating bacteria control the order and dynamics of interfacial water. <i>Science Advances</i> , 2016, 2, e1501630.	10.3	182
3	Passivating ligand and solvent contributions to the electronic properties of semiconductor nanocrystals. <i>Nanoscale</i> , 2012, 4, 904-914.	5.6	123
4	Energy-Specific Linear Response TDHF/TDDFT for Calculating High-Energy Excited States. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3540-3547.	5.3	100
5	Ab Initio Nonadiabatic Molecular Dynamics of Wet-Electrons on the TiO ₂ Surface. <i>Journal of the American Chemical Society</i> , 2009, 131, 15483-15491.	13.7	99
6	Excited State Absorption from Real-Time Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4294-4303.	5.3	70
7	Surface hopping with Ehrenfest excited potential. <i>Journal of Chemical Physics</i> , 2011, 135, 144102.	3.0	44
8	Infrared and Raman Spectroscopy from Ab Initio Molecular Dynamics and Static Normal Mode Analysis: The C-H Region of DMSO as a Case Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1429-1436.	2.6	43
9	Solvated First-Principles Excited-State Charge-Transfer Dynamics with Time-Dependent Polarizable Continuum Model and Solvent Dielectric Relaxation. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2898-2904.	4.6	40
10	Multiple Exciton Generation in Small Si Clusters: A High-Level, Ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 232-237.	4.6	38
11	Excited states and optical absorption of small semiconducting clusters: Dopants, defects and charging. <i>Chemical Science</i> , 2011, 2, 400.	7.4	38
12	Conditions for Directional Charge Transfer in CdSe Quantum Dots Functionalized by Ru(II) Polypyridine Complexes. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3565-3576.	4.6	31
13	Excited-State Absorption from Real-Time Time-Dependent Density Functional Theory: Optical Limiting in Zinc Phthalocyanine. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1387-1391.	4.6	31
14	Analysis of Correlated Dynamics in the Grotthuss Mechanism of Proton Diffusion. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5536-5544.	2.6	30
15	Trp-Cage Folding on Organic Surfaces. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10417-10425.	2.6	28
16	Correlated dynamics in aqueous proton diffusion. <i>Chemical Science</i> , 2018, 9, 7126-7132.	7.4	26
17	Non-adiabatic molecular dynamics investigation of photoionization state formation and lifetime in Mn ²⁺ -doped ZnO quantum dots. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17507.	2.8	24
18	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6418-6427.	5.3	20

#	ARTICLE	IF	CITATIONS
19	Proton transport through hydrated chitosan-based polymer membranes under electric fields. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2017, 55, 1103-1109.	2.1	9
20	Thermotropic liquid crystal (5CB) on two-dimensional materials. <i>Physical Review E</i> , 2019, 100, 062701.	2.1	7
21	Synthesis and Structure of $\text{Sn}_{14}\text{Cl}_6(\text{CH}_2\text{SiMe}_3)_{12}$: Toward Nanoclusters of 4-Coordinate $\text{I}^{\pm}\text{-Sn}$. <i>Inorganic Chemistry</i> , 2018, 57, 4921-4925.	4.0	4
22	Adsorption of the liquid crystal molecule 5CB on graphene. <i>Physical Review E</i> , 2018, 98, .	2.1	3
23	Effect of Structure and Hydration Level on Water Diffusion in Chitosan Membranes. <i>Macromolecular Theory and Simulations</i> , 2021, 30, 2000064.	1.4	2
24	Quantifying proton diffusion in acid-functionalized chitosan membranes. <i>Computational Materials Science</i> , 2022, 210, 110988.	3.0	1
25	Insertion of the Liquid Crystal 5CB into Monovacancy Graphene. <i>Molecules</i> , 2022, 27, 1664.	3.8	1