Sean A Fischer

List of Publications by Year
in descending order

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	Quantifying proton diffusion in acid-functionalized chitosan membranes. Computational Materials Science, 2022, 210, 110988.	3.0	1
2	Insertion of the Liquid Crystal 5CB into Monovacancy Graphene. Molecules, 2022, 27, 1664.	3.8	1
3	Effect of Structure and Hydration Level on Water Diffusion in Chitosan Membranes. Macromolecular Theory and Simulations, 2021, 30, 2000064.	1.4	2
4	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2020, 16, 6418-6427.	5.3	20
5	Analysis of Correlated Dynamics in the Grotthuss Mechanism of Proton Diffusion. Journal of Physical Chemistry B, 2019, 123, 5536-5544.	2.6	30
6	Thermotropic liquid crystal (5CB) on two-dimensional materials. Physical Review E, 2019, 100, 062701.	2.1	7
7	Synthesis and Structure of Sn₁₄Cl₆(CH₂SiMe₃)₁₂: Toward Nanoclusters of 4-Coordinate Î±-Sn. Inorganic Chemistry, 2018, 57, 4921-4925.	4.0	4
8	Adsorption of the liquid crystal molecule 5CB on graphene. Physical Review E, 2018, 98, .	2.1	3
9	Correlated dynamics in aqueous proton diffusion. Chemical Science, 2018, 9, 7126-7132.	7.4	26
10	Proton transport through hydrated chitosanâ€based polymer membranes under electric fields. Journal of Polymer Science, Part B: Polymer Physics, 2017, 55, 1103-1109.	2.1	9
11	Excited-State Absorption from Real-Time Time-Dependent Density Functional Theory: Optical Limiting in Zinc Phthalocyanine. Journal of Physical Chemistry Letters, 2016, 7, 1387-1391.	4.6	31
12	Ice-nucleating bacteria control the order and dynamics of interfacial water. Science Advances, 2016, 2, e1501630.	10.3	182
13	Infrared and Raman Spectroscopy from Ab Initio Molecular Dynamics and Static Normal Mode Analysis: The Câ€“H Region of DMSO as a Case Study. Journal of Physical Chemistry B, 2016, 120, 1429-1436.	2.6	43
14	Trp-Cage Folding on Organic Surfaces. Journal of Physical Chemistry B, 2015, 119, 10417-10425.	2.6	28
15	Excited State Absorption from Real-Time Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 4294-4303.	5.3	70
16	Non-adiabatic molecular dynamics investigation of photoionization state formation and lifetime in Mn²⁺-doped ZnO quantum dots. Physical Chemistry Chemical Physics, 2014, 16, 17507.	2.8	24
17	Conditions for Directional Charge Transfer in CdSe Quantum Dots Functionalized by Ru(II) Polypyridine Complexes. Journal of Physical Chemistry Letters, 2014, 5, 3565-3576.	4.6	31
18	Decoherence-induced surface hopping. Journal of Chemical Physics, 2012, 137, 22A545.	3.0	491

#	Article	IF	Citations
19	Passivating ligand and solvent contributions to the electronic properties of semiconductor nanocrystals. Nanoscale, 2012, 4, 904-914.	5.6	123
20	Solvated First-Principles Excited-State Charge-Transfer Dynamics with Time-Dependent Polarizable Continuum Model and Solvent Dielectric Relaxation. Journal of Physical Chemistry Letters, 2012, 3, 2898-2904.	4.6	40
21	Excited states and optical absorption of small semiconducting clusters: Dopants, defects and charging. Chemical Science, 2011, 2, 400.	7.4	38
22	Energy-Specific Linear Response TDHF/TDDFT for Calculating High-Energy Excited States. Journal of Chemical Theory and Computation, 2011, 7, 3540-3547.	5.3	100
23	Surface hopping with Ehrenfest excited potential. Journal of Chemical Physics, 2011, 135, 144102.	3.0	44
24	Multiple Exciton Generation in Small Si Clusters: A High-Level, Ab Initio Study. Journal of Physical Chemistry Letters, 2010, 1, 232-237.	4.6	38
25	Ab Initio Nonadiabatic Molecular Dynamics of Wet-Electrons on the TiO₂ Surface. Journal of the American Chemical Society, 2009, 131, 15483-15491.	13.7	99