Farnaz A Shakib

List of Publications by Year
in descending order

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		777949	799663
29	484	13	21
papers	citations	h-index	g-index

30	30	30	560
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Modeling energy transfer and absorption spectra in layered metal-organic frameworks based on a Frenkel-Holstein Hamiltonian. Journal of Chemical Physics, 2022, 156, 044109.	1.2	1
2	Recent progress in approximate quantum dynamics methods for the study of proton-coupled electron transfer reactions. Physical Chemistry Chemical Physics, 2021, 23, 2535-2556.	1.3	5
3	Metal-to-Semiconductor Transition in Two-Dimensional Metalâ€“Organic Frameworks: An Ab Initio Dynamics Perspective. ACS Applied Materials & Interfaces, 2021, 13, 25270-25279.	4.0	8
4	Tuning electronic properties of conductive 2D layered metalâ€“organic frameworks via hostâ€“guest interactions: Dioxygen as an electroactive chemical stimuli. APL Materials, 2021, 9, .	2.2	7
5	Gauging van der Waals interactions in aqueous solutions of 2D MOFs: when water likes organic linkers more than open-metal sites. Physical Chemistry Chemical Physics, 2021, 23, 3135-3143.	1.3	6
6	Deterministic role of structural flexibility on catalytic activity of conductive 2D layered metalâ€“organic frameworks. Chemical Communications, 2021, 57, 315-318.	2.2	6
7	Water-Induced Structural Transformations in Flexible Two-Dimensional Layered Conductive Metalâ€“Organic Frameworks. Chemistry of Materials, 2020, 32, 9664-9674.	3.2	15
8	Adsorption based realistic molecular model of amorphous kerogen. RSC Advances, 2020, 10, 23312-23320.	1.7	14
9	Optimal Separation of CO₂/CH₄/Brine with Amorphous Kerogen: A Thermodynamics and Kinetics Study. Journal of Physical Chemistry C, 2019, 123, 20877-20883.	1.5	15
10	Quasi-Diabatic Propagation Scheme for Direct Simulation of Proton-Coupled Electron Transfer Reaction. Journal of Physical Chemistry A, 2019, 123, 2470-2482.	1.1	16
11	Disentangling Coupling Effects in the Infrared Spectra of Liquid Water. Journal of Physical Chemistry B, 2018, 122, 10754-10761.	1.2	48
12	Investigating photoinduced proton coupled electron transfer reaction using quasi diabatic dynamics propagation. Journal of Chemical Physics, 2018, 148, 244102.	1.2	19
13	Ring Polymer Surface Hopping: Incorporating Nuclear Quantum Effects into Nonadiabatic Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2017, 8, 3073-3080.	2.1	47
14	New insights into the nonadiabatic state population dynamics of model proton-coupled electron transfer reactions from the mixed quantum-classical Liouville approach. Journal of Chemical Physics, 2016, 144, 024110.	1.2	11
15	Toward unsaturated stannylenes Y₂Zî€¦n: and related compounds with triplet electronic ground states. RSC Advances, 2016, 6, 53749-53759.	1.7	4
16	An analysis of model proton-coupled electron transfer reactions via the mixed quantum-classical Liouville approach. Journal of Chemical Physics, 2014, 141, 044122.	1.2	14
17	[n]Imperilenes: Stacked [n]Trannulenes Separated by Planar Cycloalkane Rings. Organic Letters, 2011, 13, 3600-3603.	2.4	3
18	Theoretical Description of Triplet Silylenes Evolved from H₂Siâ•Si. Organometallics, 2011, 30, 5027-5032.	1.1	13

#	Article	IF	Citations
19	New Generation of Dialkylsilylenes with Stabilities Comparable to Diaminosilylenes: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 10550-10555.	1.1	6
20	Isolation: A strategy for obtaining highly doped heterofullerenes. Chemical Physics Letters, 2011, 514, 321-324.	1.2	10
21	From acyclic dialkylcarbene to the unsaturated cyclic heteroatom substituted ones: a survey of stability. Journal of Physical Organic Chemistry, 2011, 24, 351-359.	0.9	14
22	Stable silylenes with acyclic, cyclic, and unsaturated cyclic structures: Effects of heteroatoms and cyclopropyl Î±-substituents at DFT. Journal of Organometallic Chemistry, 2011, 696, 2059-2064.	0.8	11
23	Stable C20â˜nSin heterofullerenes (nâ©½8): A DFT approach. Chemical Physics Letters, 2010, 492, 137-141.	1.2	25
24	Novel Î±-spirocyclic (alkyl)(amino)carbenes at the theoretical crossroad of flexibility and rigidity. Structural Chemistry, 2010, 21, 593-598.	1.0	31
25	Pyridine derived N-heterocyclic germylenes: A density functional perspective. Journal of Organometallic Chemistry, 2010, 695, 760-765.	0.8	8
26	Carbenes with Reduced Heteroatom Stabilization: A Computational Approach. Journal of Organic Chemistry, 2010, 75, 2539-2545.	1.7	47
27	A theoretical investigation into dimethylcarbene and its diamino and diphosphino analogs: effects of cyclization and unsaturation on the stability and multiplicity. Journal of Physical Organic Chemistry, 2009, 22, 919-924.	0.9	28
28	A DFT study on pyridine-derived N-heterocyclic carbenes. Tetrahedron, 2009, 65, 10093-10098.	1.0	36
29	How steric effects favor thiepins over their benzene sulfide tautomers at theoretical levels?. Computational and Theoretical Chemistry, 2008, 861, 117-121.	1.5	13