Guillaume Jeanmairet

List of Publications by Year
in descending order

25	1,073	471509	552781
papers	citations	17 h-index	26 g-index

32	32	32	1000
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Semistochastic Heat-Bath Configuration Interaction Method: Selected Configuration Interaction with Semistochastic Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 1595-1604.	5.3	232
2	Tuning water reduction through controlled nanoconfinement within an organic liquid matrix. Nature Catalysis, 2020, 3, 656-663.	34.4	91
3	Microscopic Simulations of Electrochemical Double-Layer Capacitors. Chemical Reviews, 2022, 122, 10860-10898.	47.7	81
4	Molecular Density Functional Theory of Water. Journal of Physical Chemistry Letters, 2013, 4, 619-624.	4.6	76
5	Fast Computation of Solvation Free Energies with Molecular Density Functional Theory: Thermodynamic-Ensemble Partial Molar Volume Corrections. Journal of Physical Chemistry Letters, 2014, 5, 1935-1942.	4.6	67
6	Solvation free-energy pressure corrections in the three dimensional reference interaction site model. Journal of Chemical Physics, 2015, 143, 184116.	3.0	67
7	MetalWalls: A classical molecular dynamics software dedicated to the simulation of electrochemical systems. Journal of Open Source Software, 2020, 5, 2373.	4.6	56
8	Capacitive Performance of Water-in-Salt Electrolytes in Supercapacitors: A Simulation Study. Journal of Physical Chemistry C, 2018, 122, 23917-23924.	3.1	49
9	Simulating Electrochemical Systems by Combining the Finite Field Method with a Constant Potential Electrode. Physical Review Letters, 2019, 123, 195501.	7.8	48
10	Extension of Marcus Picture for Electron Transfer Reactions with Large Solvation Changes. Journal of the American Chemical Society, 2012, 134, 2067-2074.	13.7	42
11	Molecular density functional theory of water describing hydrophobicity at short and long length scales. Journal of Chemical Physics, 2013, 139, 154101.	3.0	37
12	Study of a water-graphene capacitor with molecular density functional theory. Journal of Chemical Physics, 2019, 151, 124111.	3.0	31
13	Confinement Effects on an Electron Transfer Reaction in Nanoporous Carbon Electrodes. Journal of Physical Chemistry Letters, 2017, 8, 1925-1931.	4.6	29
14	Molecular density functional theory for water with liquid-gas coexistence and correct pressure. Journal of Chemical Physics, 2015, 142, 154112.	3.0	26
15	A molecular density functional theory approach to electron transfer reactions. Chemical Science, 2019, 10, 2130-2143.	7.4	24
16	Solvation of complex surfaces via molecular density functional theory. Journal of Chemical Physics, 2012, 137, 224107.	3.0	23
17	Tackling Solvent Effects by Coupling Electronic and Molecular Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 7123-7134.	5.3	19
18	Molecular density functional theory of water including densityâ€“polarization coupling. Journal of Physics Condensed Matter, 2016, 28, 244005.	1.8	15

#	Article	IF	Citations
19	Simple Parameter-Free Bridge Functionals for Molecular Density Functional Theory. Application to Hydrophobic Solvation. Journal of Physical Chemistry B, 2020, 124, 6885-6893.	2.6	13
20	Hydration of clays at the molecular scale: the promising perspective of classical density functional theory. Molecular Physics, 2014, 112, 1320-1329.	1.7	11
21	Accurate prediction of hydration free energies and solvation structures using molecular density functional theory with a simple bridge functional. Journal of Chemical Physics, 2021, 155, 024117.	3.0	9
22	Introduction to Classical Density Functional Theory by a Computational Experiment. Journal of Chemical Education, 2014, 91, 2112-2115.	2.3	8
23	A first-principles investigation of the structural and electrochemical properties of biredox ionic species in acetonitrile. Physical Chemistry Chemical Physics, 2020, 22, 10561-10568.	2.8	8
24	Multi-scale simulation of the adsorption of lithium ion on graphite surface: From quantum Monte Carlo to molecular density functional theory. Journal of Chemical Physics, 2022, 156, 094709.	3.0	6
25	Assessing the correctness of pressure correction to solvation theories in the study of electron transfer reactions. Journal of Chemical Physics, 2021, 154, 131102.	3.0	3