Elise DubouÃ©-Dijon

List of Publications by Year
in descending order

18	878	706676 14	939365 18
papers	citations	h-index	g-index

29	29	29	1409
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Building intuition for binding free energy calculations: Bound state definition, restraints, and symmetry. Journal of Chemical Physics, 2021, 154, 204101.	1.2	22
2	Binding of divalent cations to acetate: molecular simulations guided by Raman spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 24014-24027.	1.3	28
3	A practical guide to biologically relevant molecular simulations with charge scaling for electronic polarization. Journal of Chemical Physics, 2020, 153, 050901.	1.2	63
4	Quantifying the Strength of a Salt Bridge by Neutron Scattering and Molecular Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 3254-3259.	2.1	14
5	Calcium ions in aqueous solutions: Accurate force field description aided by ab initio molecular dynamics and neutron scattering. Journal of Chemical Physics, 2018, 148, 222813.	1.2	75
6	Binding of Divalent Cations to Insulin: Capillary Electrophoresis and Molecular Simulations. Journal of Physical Chemistry B, 2018, 122, 5640-5648.	1.2	45
7	Hydration and Ion Pairing in Aqueous Mg²⁺ and Zn²⁺ Solutions: Force-Field Description Aided by Neutron Scattering Experiments and Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 3296-3306.	1.2	75
8	Can Arginine Inhibit Insulin Aggregation? A Combined Protein Crystallography, Capillary Electrophoresis, and Molecular Simulation Study. Journal of Physical Chemistry B, 2018, 122, 10069-10076.	1.2	28
9	Ab Initio Simulations of Water Dynamics in Aqueous TMAO Solutions: Temperature and Concentration Effects. Journal of Physical Chemistry B, 2017, 121, 11189-11197.	1.2	24
10	Changes in the hydration structure of imidazole upon protonation: Neutron scattering and molecular simulations. Journal of Chemical Physics, 2017, 146, .	1.2	14
11	Coupled Valence-Bond State Molecular Dynamics Description of an Enzyme-Catalyzed Reaction in a Non-Aqueous Organic Solvent. Journal of Physical Chemistry B, 2017, 121, 7027-7041.	1.2	11
12	Dynamical Disorder in the DNA Hydration Shell. Journal of the American Chemical Society, 2016, 138, 7610-7620.	6.6	103
13	Characterization of the Local Structure in Liquid Water by Various Order Parameters. Journal of Physical Chemistry B, 2015, 119, 8406-8418.	1.2	153
14	Comparative study of hydration shell dynamics around a hyperactive antifreeze protein and around ubiquitin. Journal of Chemical Physics, 2014, 141, 22D529.	1.2	50
15	Origins of the non-exponential reorientation dynamics of nanoconfined water. Journal of Chemical Physics, 2014, 141, 18C523.	1.2	36
16	Temperature Dependence of Hydrophobic Hydration Dynamics: From Retardation to Acceleration. Journal of Physical Chemistry B, 2014, 118, 1574-1583.	1.2	34
17	Biomolecular hydration dynamics: a jump model perspective. Chemical Society Reviews, 2013, 42, 5672.	18.7	100
18	Consistent Picture of Phosphateâ€“Divalent Cation Binding from Models with Implicit and Explicit Electronic Polarization. Journal of Physical Chemistry B, 0, , .	1.2	1