Gregory R Medders

List of Publications by Year in Descending Order

13 papers	1,109 citations	10 h-index	14 g-index
14 ext. papers	1,268 ext. citations	6.2 avg, IF	4.95 L-index

#	Paper	IF	Citations
13	Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model.. *Journal of Physical Chemistry Letters*, **2022**, 3652-3658	6.4	4
12	Configuration interaction singles with spin-orbit coupling: Constructing spin-adiabatic states and their analytical nuclear gradients. *Journal of Chemical Physics*, **2019**, 150, 014106	3.9	9
11	Ultrafast Electronic Relaxation through a Conical Intersection: Nonadiabatic Dynamics Disentangled through an Oscillator Strength-Based Diabatization Framework. *Journal of Physical Chemistry A*, **2017**, 121, 1425-1434	2.8	10
10	Dissecting the Molecular Structure of the Air/Water Interface from Quantum Simulations of the Sum-Frequency Generation Spectrum. *Journal of the American Chemical Society*, **2016**, 138, 3912-9	16.4	116
9	On the interplay of the potential energy and dipole moment surfaces in controlling the infrared activity of liquid water. *Journal of Chemical Physics*, **2015**, 142, 212411	3.9	27
8	On the representation of many-body interactions in water. *Journal of Chemical Physics*, **2015**, 143, 104102	3.9	74
7	Infrared and Raman Spectroscopy of Liquid Water through "First-Principles" Many-Body Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 1145-54	6.4	125
6	Water Dynamics in Metal-Organic Frameworks: Effects of Heterogeneous Confinement Predicted by Computational Spectroscopy. *Journal of Physical Chemistry Letters*, **2014**, 5, 2897-902	6.4	37
5	Development of a "First Principles" Water Potential with Flexible Monomers. II: Trimer Potential Energy Surface, Third Virial Coefficient, and Small Clusters. *Journal of Chemical Theory and Computation*, **2014**, 10, 1599-607	6.4	230
4	Development of a "First-Principles" Water Potential with Flexible Monomers. III. Liquid Phase Properties. *Journal of Chemical Theory and Computation*, **2014**, 10, 2906-10	6.4	227
3	Many-Body Convergence of the Electrostatic Properties of Water. *Journal of Chemical Theory and Computation*, **2013**, 9, 4844-52	6.4	24
2	A Critical Assessment of Two-Body and Three-Body Interactions in Water. *Journal of Chemical Theory and Computation*, **2013**, 9, 1103-14	6.4	111
1	Toward a Universal Water Model: First Principles Simulations from the Dimer to the Liquid Phase. *Journal of Physical Chemistry Letters*, **2012**, 3, 3765-9	6.4	114