Rafael R Pappalardo

List of Publications by Year
in descending order

30 papers	956 citations	471509 17 h-index	454955 30 g-index
30 all docs	30 docs citations	30 times ranked	740 citing authors

#	Article	IF	Citations
1	First-Principles Ionâ^'Water Interaction Potentials for Highly Charged Monatomic Cations. Computer Simulations of Al3+, Mg2+, and Be2+in Water. Journal of the American Chemical Society, 1999, 121, 3175-3184.	13.7	123
2	Effects of the solvent reaction field on the geometrical structures of hexahydrate metallic cations. The Journal of Physical Chemistry, 1991, 95, 8928-8932.	2.9	84
3	Recovering the concept of the hydrated ion for modeling ionic solutions: a Monte Carlo study of zinc(2+) in water. The Journal of Physical Chemistry, 1993, 97, 4500-4504.	2.9	72
4	Solving the Hydration Structure of the Heaviest Actinide Aqua Ion Known: The Californium(III) Case. Angewandte Chemie - International Edition, 2010, 49, 3811-3815.	13.8	64
5	Understanding the Hydration Structure of Square-Planar Aquaions:Â The [Pd(H2O)4]2+Case. Journal of Physical Chemistry B, 2004, 108, 15851-15855.	2.6	56
6	Application of the Hydrated Ion Concept for Modeling Aqueous Solutions Containing Highly Charged Ions:Â A Monte Carlo Simulation of Cr3+in Water Using an ab Initio Intermolecular Potentialâ€. The Journal of Physical Chemistry, 1996, 100, 11748-11754.	2.9	53
7	A molecular dynamics study of the Cr3+ hydration based on a fully flexible hydrated ion model. Journal of Chemical Physics, 1998, 109, 1445-1455.	3.0	49
8	The hydration structure of the heavy-alkalines Rb⁺ and Cs⁺ through molecular dynamics and X-ray absorption spectroscopy: surface clusters and eccentricity. Physical Chemistry Chemical Physics, 2017, 19, 28993-29004.	2.8	43
9	Analysis of the Opposite Solvent Effects Caused by Different Solute Cavities on the Metalâ^'Water Distance of Monoatomic Cation Hydrates. Journal of Physical Chemistry B, 2002, 106, 1118-1123.	2.6	42
10	Dynamics of a Highly Charged Ion in Aqueous Solutions:Â MD Simulations of Dilute CrCl3Aqueous Solutions Using Interaction Potentials Based on the Hydrated Ion Concept. Journal of Physical Chemistry B, 1998, 102, 3272-3282.	2.6	41
11	Combined Experimental and Theoretical Approach to the Study of Structure and Dynamics of the Most Inert Aqua Ion [Ir(H2O)6]3+in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 8223-8233.	2.6	38
12	Hydration Structure and Dynamic Properties of the Square Planar Pt(II) Aquaion Compared to the Pd(II) Case. Theoretical Chemistry Accounts, 2006, 115, 196-203.	1.4	34
13	Aqueous Pd^{II} and Pt^{II}: Anionic Hydration Revealed by Carâ€"Parrinello Simulations. ChemPhysChem, 2008, 9, 237-240.	2.1	32
14	Hydration of Two Cisplatin Aqua-Derivatives Studied by Quantum Mechanics and Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 1735-1744.	5.3	28
15	Hydration of Cisplatin Studied by an Effective Ab Initio Pair Potential Including Soluteâ€"Solvent Polarization. Journal of Chemical Theory and Computation, 2013, 9, 4562-4573.	5.3	27
16	Identifying Coordination Geometries of Metal Aquaions in Water: Application to the Case of Lanthanoid and Actinoid Hydrates. Journal of Physical Chemistry Letters, 2016, 7, 4275-4280.	4.6	25
17	Collecting high-order interactions in an effective pairwise intermolecular potential using the hydrated ion concept: The hydration of Cf3+. Journal of Chemical Physics, 2014, 140, 214104.	3.0	18
18	An Ab Initio Molecular Dynamics Study on the Hydrolysis of the Po(IV) Aquaion in Water. Journal of Physical Chemistry B, 2010, 114, 12866-12874.	2.6	17

#	Article	IF	Citations
19	A hydrated ion model of [UO2]2+ in water: Structure, dynamics, and spectroscopy from classical molecular dynamics. Journal of Chemical Physics, 2016, 145, 224502.	3.0	17
20	General Quantum-Mechanical Study on the Hydrolysis Equilibria for a Tetravalent Aquaion: The Extreme Case of the Po(IV) in Water. Journal of Physical Chemistry B, 2009, 113, 487-496.	2.6	14
21	Hydration Structure of the Elusive Ac(III) Aqua Ion: Interpretation of X-ray Absorption Spectroscopy (XAS) Spectra on the Basis of Molecular Dynamics (MD) Simulations. Inorganic Chemistry, 2019, 58, 2777-2783.	4.0	14
22	A general study of actinyl hydration by molecular dynamics simulations using ab initio force fields. Journal of Chemical Physics, 2019, 150, 104504.	3.0	13
23	Effect of Basicity on the Hydrolysis of the Bi(III) Aqua Ion in Solution: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry A, 2018, 122, 1905-1915.	2.5	12
24	Extracting the Americyl Hydration from an Americium Cationic Mixture in Solution: A Combined X-ray Absorption Spectroscopy and Molecular Dynamics Study. Inorganic Chemistry, 2018, 57, 8089-8097.	4.0	9
25	Hydration of Heavy Alkaline-Earth Cations Studied by Molecular Dynamics Simulations and X-ray Absorption Spectroscopy. Inorganic Chemistry, 2021, 60, 13578-13587.	4.0	9
26	Quantum-Mechanical Study on the Aquaions and Hydrolyzed Species of Po(IV), Te(IV), and Bi(III) in Water. Journal of Physical Chemistry B, 2012, 116, 14903-14914.	2.6	7
27	Revisiting the cobalt(II) hydration from molecular dynamics and X-ray absorption spectroscopy. Molecular Physics, 2019, 117, 3320-3328.	1.7	5
28	A Coupled EXAFSâ€“Molecular Dynamics Study on PuO₂⁺ and NpO₂⁺ Hydration: The Importance of Electron Correlation in Force-Field Building. Inorganic Chemistry, 2022, 61, 8703-8714.	4.0	5
29	Development of a polarizable and flexible model of the hydrated ion potential to study the intriguing case of Sc(III) hydration. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	3
30	Combining EXAFS and Computer Simulations to Refine the Structural Description of Actinyls in Water. Molecules, 2020, 25, 5250.	3.8	2