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	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
2	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
3	Combining EXAFS and Computer Simulations to Refine the Structural Description of Actinyls in Water. Molecules, 2020, 25, 5250.	3.8	2
4	Revisiting the cobalt(II) hydration from molecular dynamics and X-ray absorption spectroscopy. Molecular Physics, 2019, 117, 3320-3328.	1.7	5
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	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
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	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
17	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
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	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
20	Aqueous Pd^{II} and Pt^{II}: Anionic Hydration Revealed by Carâ€“Parrinello Simulations. ChemPhysChem, 2008, 9, 237-240.	2.1	32
21	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
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	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