Enrique Sanchez Marcos

List of Publications by Year
in descending order

113	3,131	117625	182427
papers	citations	34 h-index	51 g-index

117	117	117	2354
all docs	docs citations	times ranked	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	A general purpose acetonitrile interaction potential to describe its liquid, solid and gas phases. Journal of Molecular Liquids, 2020, 318, 113975.	4.9	4
5	Revisiting the cobalt(II) hydration from molecular dynamics and X-ray absorption spectroscopy. Molecular Physics, 2019, 117, 3320-3328.	1.7	5
6	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
7	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
8	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
9	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
10	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
11	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
12	Hydration and Diffusion Mechanism of Uranyl in Montmorillonite Clay: Molecular Dynamics Using an Ab Initio Potential. Journal of Physical Chemistry C, 2017, 121, 27437-27444.	3.1	16
13	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
14	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
15	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
16	Theoretical study on the hydrophobic and hydrophilic hydration on large solutes: The case of phthalocyanines in water. Journal of Chemical Physics, 2015, 143, 044502.	3.0	3
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	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

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19	Molecular Structure of Solvates and Coordination Complexes in Solution as Determined with EXAFS and XANES. , 2013, , 133-159.		8
20	EXAFS Debye-Waller factors issued from Car-Parrinello molecular dynamics: Application to the fit of oxaliplatin and derivatives. Journal of Chemical Physics, 2013, 138, 084303.	3.0	9
21	Impact of the number of fitted Debye-Waller factors on EXAFS fitting. Journal of Physics: Conference Series, 2013, 430, 012015.	0.4	9
22	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
23	Axial Structure of the Pd(II) Aqua Ion in Solution. Journal of the American Chemical Society, 2012, 134, 962-967.	13.7	50
24	Modeling the interactions of phthalocyanines in water: From the Cu(II)-tetrasulphonate to the metal-free phthalocyanine. Journal of Chemical Physics, 2011, 134, 024503.	3.0	3
25	Comparative study of the hydrolysis of a third- and a first-generation platinum anticancer complexes. Theoretical Chemistry Accounts, 2011, 128, 627-638.	1.4	36
26	Theoretical and computational chemistry in Spain. Theoretical Chemistry Accounts, 2011, 128, 389-391.	1.4	0
27	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
28	Molecular solids of actinide hexacyanoferrate: Structure and bonding. IOP Conference Series: Materials Science and Engineering, 2010, 9, 012026.	0.6	2
29	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
30	A theoretical study of the hydrogen bond donor capability and co-operative effects in the hydrogen bond complexes of the diaza-aromatic betacarbolines. Physical Chemistry Chemical Physics, 2010, 12, 5276.	2.8	9
31	Characterizing Ptâ€Đerived Anticancer Drugs from First Principles: The Case of Oxaliplatin in Aqueous Solution. ChemPhysChem, 2009, 10, 1044-1052.	2.1	23
32	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
33	Coupling CP-MD Simulations and X-ray Absorption Spectroscopy: Exploring the Structure of Oxaliplatin in Aqueous Solution. Journal of Physical Chemistry B, 2009, 113, 12343-12352.	2.6	20
34	Opposite effects of successive hydration shells on the aqua ion structure of metal cations. Molecular Simulation, 2009, 35, 1007-1014.	2.0	4
35	Aqueous Pd^{II} and Pt^{II}: Anionic Hydration Revealed by Carâ€“Parrinello Simulations. ChemPhysChem, 2008, 9, 237-240.	2.1	32
36	Po(IV) Hydration:â€‰ A Quantum Chemical Study. Journal of Physical Chemistry B, 2008, 112, 5416-5422.	2.6	21

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37	Explaining Asymmetric Solvation of Pt(II) versus Pd(II) in Aqueous Solution Revealed by Ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2008, 4, 2108-2121.	5.3	56
38	Coupling MD Simulations and X-ray Absorption Spectroscopy to Study Ions in Solution. AIP Conference Proceedings, 2007, , .	0.4	0
39	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
40	The Aquation of Po(IV): A Quantum Chemical Study.. AIP Conference Proceedings, 2007, , .	0.4	1
41	Coupling MD Simulations and X-ray Absorption Spectroscopy to Study Ions in Solution. AIP Conference Proceedings, 2007, , .	0.4	0
42	The hydration of Cu2+: Can the Jahn-Teller effect be detected in liquid solution?. Journal of Chemical Physics, 2006, 124, 064509.	3.0	104
43	The interplay of the 3d9and 3d10underline{i{L}} electronic configurations in the copperK-edge XANES spectra of Cu(II) compounds. Journal of Synchrotron Radiation, 2006, 13, 471-476.	2.4	19
44	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
45	Theoretical chemistry of metal and single ions in solutions. Theoretical Chemistry Accounts, 2006, 115, 75-76.	1.4	1
46	Analysis of Main Factors Determining the Prediction of Stabilization Energies of Halide-water Clusters. Theoretical Chemistry Accounts, 2006, 116, 691-699.	1.4	3
47	The solvation of bromide anion in acetonitrile: a structural study based on the combination of theoretical calculations and X-ray absorption spectroscopy. Molecular Simulation, 2006, 32, 1035-1043.	2.0	7
48	Ab initiox-ray absorption study of copperK-edge XANES spectra in Cu(II) compounds. Physical Review B, 2005, 71, .	3.2	82
49	Study of the stabilization energies of halide-water clusters: An application of first-principles interaction potentials based on a polarizable and flexible model. Journal of Chemical Physics, 2004, 121, 7269-7275.	3.0	25
50	A molecular dynamics study on Rh3+ hydration: development and application of a first principles hydrated ionâ€“water interaction potential. Theoretical Chemistry Accounts, 2004, 111, 101-109.	1.4	7
51	Unterstanding the Hydration Structure of Square-Planar Aquaions: The [Pd(H2O)4]2+ Case. ChemInform, 2004, 35, no.	0.0	0
52	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
53	Nature of Metal Binding Sites in Cu(II) Complexes with Histidine and Related N-Coordinating Ligands, As Studied by EXAFS. Inorganic Chemistry, 2004, 43, 6674-6683.	4.0	61
54	On the halide hydration study: Development of first-principles halide ion-water interaction potential based on a polarizable model. Journal of Chemical Physics, 2003, 119, 9538-9548.	3.0	61

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55	Interplay of computer simulations and x-ray absorption spectra in the study of the bromide hydration structure. Journal of Chemical Physics, 2003, 119, 6647-6654.	3.0	33
56	Development of first-principles interaction model potentials. An application to the study of the bromide hydration. Journal of Chemical Physics, 2002, 117, 10512-10524.	3.0	40
57	Exploring the Capabilities of X-ray Absorption Spectroscopy for Determining the Structure of Electrolyte Solutions:â€‰ Computed Spectra for Cr3+ or Rh3+ in Water Based on Molecular Dynamics. Journal of the American Chemical Society, 2002, 124, 10911-10920.	13.7	72
58	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
59	Geometry and Hydration Structure of Pt(II) Square Planar Complexes [Pt(H2O)4]2+and [PtCl4]2-as Studied by X-ray Absorption Spectroscopies and Quantum-Mechanical Computations. Journal of Physical Chemistry B, 2001, 105, 7588-7593.	2.6	71
60	Combination of XANES spectroscopy and molecular dynamics to probe the local structure in disordered systems. Physical Review B, 2001, 64, .	3.2	38
61	Molecular-dynamics-based investigation of scattering path contributions to the EXAFS spectrum: TheCr3+aqueous solution case. Physical Review B, 2001, 64, .	3.2	28
62	Unusual spectroscopic behaviour of the carbonyl and carbonâ€“carbon double-bond groups in the infrared spectra of simple nitroenaminoketone derivatives. Chemical Physics Letters, 2000, 323, 400-406.	2.6	5
63	Coupling a polarizable water model to the hydrated ionâ€“water interaction potential: A test on the Cr3+ hydration. Journal of Chemical Physics, 2000, 112, 2339-2347.	3.0	42
64	Importance of Multiple-Scattering Phenomena in XAS Structural Determinations of [Ni(CN)4]2-in Condensed Phases. Inorganic Chemistry, 2000, 39, 3784-3790.	4.0	22
65	Theoretical Study of the Microsolvation of the Bromide Anion in Water, Methanol, and Acetonitrile:Â Ionâ^'Solvent vs Solventâ^'Solvent Interactions. Journal of Physical Chemistry A, 2000, 104, 2799-2807.	2.5	72
66	X-ray Absorption Spectroscopy Study of the In-Solution Structure of Ni2+, Co2+, and Ag+ Solvates in Acetonitrile Including Multiple Scattering Contributions. Journal of Physical Chemistry B, 2000, 104, 11794-11800.	2.6	19
67	Shape and size of simple cations in aqueous solutions: A theoretical reexamination of the hydrated ion via computer simulations. Journal of Chemical Physics, 1999, 110, 1669-1676.	3.0	11
68	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
69	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
70	Second Hydration Shell Single Scattering versus First Hydration Shell Multiple Scattering in M(H2O)63+EXAFS Spectra. Journal of the American Chemical Society, 1998, 120, 10397-10401.	13.7	53
71	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
72	Response to â€œComment on â€˜Examining the influence of the [Zn(H2O)6]2+ geometry change on the Monte Carlo simulations of Zn2+ in waterâ€™â€‰â€•[J. Chem. Phys. 108, 1750 (1998)]. Journal of Chemical Physics, 1998, 108, 1752-1753.	3.0	7

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73	An Experimental and Theoretical Study on the Prototropic Equilibria of the Four Carboline Isomers. Journal of Organic Chemistry, 1997, 62, 5104-5109.	3.2	17
74	Study of the Ag+ Hydration by Means of a Semicontinuum Quantum-Chemical Solvation Model. Journal of Physical Chemistry A, 1997, 101, 4444-4448.	2.5	64
75	EXAFS Study of the Hydration Structure of Ga Aqueous Solution. Comparison of Data from two Laboratories. European Physical Journal Special Topics, 1997, 7, C2-647-C2-648.	0.2	2
76	EXAFS Investigation of Inner- and Outer-Sphere Chloroaquo Complexes of Cr3+in Aqueous Solutions. Journal of the American Chemical Society, 1996, 118, 12654-12664.	13.7	40
77	Role of geometrical relaxation in solution of simple molecules exhibiting anomeric effects. Computational and Theoretical Chemistry, 1996, 371, 245-256.	1.5	17
78	Examining the influence of the [Zn(H2O)6]2+ geometry change on the Monte Carlo simulations of Zn2+ in water. Journal of Chemical Physics, 1996, 105, 5968-5970.	3.0	26
79	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
80	Design of an EXAFS cell for measurements of ionic solutions in a wide range of concentrations and in highly acidic media. Physica B: Condensed Matter, 1995, 208-209, 241-242.	2.7	6
81	EXAFS investigation of the second hydration shell of metal cations in dilute aqueous solutions. Physica B: Condensed Matter, 1995, 208-209, 395-397.	2.7	12
82	Determination of the Second Hydration Shell of Cr3+ and Zn2+ in Aqueous Solutions by Extended X-ray Absorption Fine Structure. Journal of the American Chemical Society, 1995, 117, 11710-11720.	13.7	101
83	Calculation of the Weights of Resonance Structures of Molecules in Solution. The Journal of Physical Chemistry, 1995, 99, 6461-6467.	2.9	32
84	Liquid EXAFS cells for measurements in transmission and fluorescence mode of corrosive samples. Review of Scientific Instruments, 1994, 65, 2153-2154.	1.3	30
85	Natural polyelectron population analysis. International Journal of Quantum Chemistry, 1994, 52, 1127-1144.	2.0	36
86	Geometrical structure of the cis- and trans-isomers of 1,2-dihaloethylenes and the energetics of their chemical equilibrium in solution. Chemical Physics Letters, 1994, 225, 202-207.	2.6	9
87	Examination of the Hund rule in closed-shell systems: Investigation of spin correlation effects. International Journal of Quantum Chemistry, 1993, 47, 191-211.	2.0	17
88	Solvent effects on molecular geometries and isomerization processes: a study of push-pull ethylenes in solution. Journal of the American Chemical Society, 1993, 115, 3722-3730.	13.7	85
89	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
90	Theoretical suggestion for the aquazinc(2+) formation. The Journal of Physical Chemistry, 1992, 96, 516-518.	2.9	16

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91	Three-center four-electron bonds and their indices. Chemical Physics Letters, 1992, 192, 14-20.	2.6	79
92	Experimental evidence by EXAFS of the second hydration shell in dilute solutions of chromium(III) ion. Journal of the American Chemical Society, 1992, 114, 6931-6932.	13.7	24
93	Investigating the possibility of simultaneously finding an electron-hole and an electron-pair in a molecule: Delocalization, competition of ionic vs. covalent character, and related effects in push-pull ethylenes. International Journal of Quantum Chemistry, 1992, 44, 337-362.	2.0	27
94	Theoretical approach to the solvation of nitroenamines and the influence of solvation on isomeric equilibria. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1719.	1.7	11
95	AM1 study of a Î²-carboline set. Part III: substituent effects. Journal of the Chemical Society Perkin Transactions II, 1991, , 1729-1734.	0.9	18
96	Theoretical study of simple push-pull ethylenes in solution. Journal of Physical Organic Chemistry, 1991, 4, 141-148.	1.9	29
97	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
98	MNDO and AM1 estimation of the electrostatic, induction and dispersion contributions to the solvation energy by a continuum model. Computational and Theoretical Chemistry, 1990, 210, 441-446.	1.5	6
99	H2 chemisorption on Ir4 clusters: A HFS-LCAO study. Chemical Physics Letters, 1990, 167, 399-406.	2.6	49
100	AM1 study of a Î²-carboline set: structural properties and potential reactivity. Journal of the Chemical Society Perkin Transactions II, 1990, , 65-71.	0.9	32
101	AM1 Study of a Î²-carboline set. Part II: pyrrole-N deprotonated species. Journal of the Chemical Society Perkin Transactions II, 1990, , 1881-1884.	0.9	15
102	A theoretical approach to the vibrational analysis of the nitroenamine system. Journal of the Chemical Society Perkin Transactions II, 1990, , 1627-1636.	0.9	5
103	Electron-pair distributions in the carbon-carbon double bond: effects of a push-pull substitution. The Journal of Physical Chemistry, 1990, 94, 2763-2767.	2.9	31
104	Spectral properties and isomerism of nitro enamines. Part 2. 3-Amino-2-nitrocrotonic esters. Journal of the Chemical Society Perkin Transactions II, 1990, , 385-392.	0.9	11
105	Effect of diffuse functions on the potential-energy surfaces of the alkylation reactions Xâ€“+ CH3F â†' XCH3+ Fâ€“(X = OH, CH3, H2CCHO). Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1531-1538.	1.1	4
106	MNDO/H and AM1 studies of nitro enamines with intramolecular hydrogen bonds. Journal of the Chemical Society Perkin Transactions II, 1988, , 2059-2064.	0.9	13
107	Ab initio study of stable bis(carbon dioxide)molybdenum complexes. Journal of the Chemical Society Dalton Transactions, 1987, , 2373.	1.1	9
108	Theoretical study of the different coordination modes of copper-carbon dioxide complex. The Journal of Physical Chemistry, 1987, 91, 1328-1333.	2.9	63

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109	Electrostatic interactions as a factor in the determination of the HOMO in the liquid state. Canadian Journal of Chemistry, 1986, 64, 2353-2358.	1.1	18
110	The second step of the BAC2 mechanism for neutral esters: a theoretical study. Journal of the Chemical Society Perkin Transactions II, 1986, , 1323-1325.	0.9	6
111	Protonation of nitrogen-containing bases in solution: continuum vs. discrete-continuum models for aqueous solutions. The Journal of Physical Chemistry, 1985, 89, 4695-4700.	2.9	56
112	IONPIT: A full implementation of Pitzer's ion interaction treatment. Computers & Chemistry, 1985, 9, 185-190.	1.2	1
113	Activity coefficients of zinc chloride in the presence of lithium, sodium, and magnesium perchlorates, and magnesium nitrate in aqueous solution at 25ï¿½C. Journal of Solution Chemistry, 1982, 11, 889-896.	1.2	1