Carine Clavaguera

List of Publications by Year
in descending order

76	1,877	218677	289244
papers	citations	26 h-index	40 g-index

83	83	83	1823
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Predicted Organometallic Series Following a 32-Electron Principle: An@C₂₈(An = Th,) Tj ETQq1 1 0.784314 rgBT /Over 131, 238-243.	13.7	106
2	Towards a 32-Electron Principle: Pu@Pb12 and Related Systems. Angewandte Chemie - International Edition, 2007, 46, 1427-1430.	13.8	88
3	Can density functional methods be used for open-shell actinide molecules? Comparison with multiconfigurational spin-orbit studies. Journal of Chemical Physics, 2004, 121, 5312-5321.	3.0	81
4	Molecular Dynamics Study of the Hydration of Lanthanum(III) and Europium(III) Including Many-Body Effects. Journal of Physical Chemistry B, 2005, 109, 7614-7616.	2.6	79
5	Modeling of Uranyl Cationâ^'Water Clusters. Journal of Physical Chemistry B, 2003, 107, 3051-3060.	2.6	76
6	Calculated lanthanide contractions for molecular trihalides and fully hydrated ions: The contributions from relativity and 4f-shell hybridization. Chemical Physics Letters, 2006, 429, 8-12.	2.6	71
7	Toward accurate solvation dynamics of lanthanides and actinides in water using polarizable force fields: from gas-phase energetics to hydration free energies. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	62
8	Theoretical study of the hydrated Gd3+ ion: Structure, dynamics, and charge transfer. Journal of Chemical Physics, 2006, 124, 074505.	3.0	56
9	Modeling Complexes of the Uranyl Ion UO2L2n+:â€‰ Binding Energies, Geometries, and Bonding Analysis. Journal of Physical Chemistry A, 2003, 107, 4515-4525.	2.5	52
10	Lanthanidocenes: Synthesis, Structure, and Bonding of Linear Sandwich Complexes of Lanthanides. Journal of the American Chemical Society, 2018, 140, 14433-14439.	13.7	50
11	Structure of sodiated octa-glycine: IRMPD spectroscopy and molecular modeling. Journal of the American Society for Mass Spectrometry, 2010, 21, 728-738.	2.8	45
12	A new, centered 32-electron system: the predicted [U@Si20]6â^'-like isoelectronic series. Chemical Science, 2012, 3, 2843.	7.4	42
13	Simulating Electron Dynamics in Polarizable Environments. Journal of Chemical Theory and Computation, 2017, 13, 3985-4002.	5.3	41
14	Calculation of harmonic and anharmonic vibrational wavenumbers for triatomic uranium compounds XUY. Chemical Physics, 2004, 302, 1-11.	1.9	36
15	Hydration gibbs free energies of open and closed shell trivalent lanthanide and actinide cations from polarizable molecular dynamics. Journal of Molecular Modeling, 2014, 20, 2471.	1.8	35
16	Theoretical Insights into the Nature of Divalent Lanthanideâ€“Ligand Interactions. Organometallics, 2013, 32, 1265-1271.	2.3	34
17	IRMPD Spectroscopy of a Protonated, Phosphorylated Dipeptide. ChemPhysChem, 2008, 9, 2564-2573.	2.1	33
18	Globule to Helix Transition in Sodiated Polyalanines. Journal of Physical Chemistry Letters, 2012, 3, 3320-3324.	4.6	33

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19	Structures and IR Spectra of the Gramicidin S Peptide: Pushing the Quest for Low-Energy Conformations. Journal of Physical Chemistry B, 2012, 116, 483-490.	2.6	33
20	Accurate static electric dipole polarizability calculations of +3 charged lanthanide ions. Chemical Physics, 2005, 311, 169-176.	1.9	32
21	Tuning the Stability of Pd(IV) Intermediates Using a Redox Non-innocent Ligand Combined with an Organolanthanide Fragment. Journal of the American Chemical Society, 2017, 139, 10633-10636.	13.7	32
22	Ab Initio Extension of the AMOEBA Polarizable Force Field to Fe²⁺. Journal of Chemical Theory and Computation, 2013, 9, 3062-3071.	5.3	31
23	Multiple One-Electron Transfers in Bipyridine Complexes of Bis(phospholyl) Thulium. Organometallics, 2014, 33, 4100-4106.	2.3	31
24	Assessing cluster models of solvation for the description of vibrational circular dichroism spectra: synergy between static and dynamic approaches. Physical Chemistry Chemical Physics, 2020, 22, 26047-26068.	2.8	31
25	Reductive Disproportionation of CO₂ with Bulky Divalent Samarium Complexes. Organometallics, 2017, 36, 4660-4668.	2.3	30
26	Chirality-dependent structuration of protonated or sodiated polyphenylalanines: IRMPD and ion mobility studies. Physical Chemistry Chemical Physics, 2016, 18, 1807-1817.	2.8	27
27	Bisâ€Cyclooctatetraenyl Thulium(II): Highly Reducing Lanthanide Sandwich Singleâ€Molecule Magnets. Angewandte Chemie - International Edition, 2021, 60, 6042-6046.	13.8	27
28	Chemical properties of the predicted 32-electron systems Pu@Sn12 and Pu@Pb12. Comptes Rendus Chimie, 2010, 13, 884-888.	0.5	26
29	Free Energy Simulations of a GTPase: GTP and GDP Binding to Archaeal Initiation Factor 2. Journal of Physical Chemistry B, 2011, 115, 6749-6763.	2.6	26
30	Assessment of Density Functionals for Computing Thermodynamic Properties of Lanthanide Complexes. ChemPhysChem, 2017, 18, 2688-2696.	2.1	25
31	Divalent Thulium Triflate: A Structural and Spectroscopic Study. Angewandte Chemie - International Edition, 2017, 56, 4266-4271.	13.8	24
32	Finite Temperature Infrared Spectra from Polarizable Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 3190-3199.	5.3	23
33	Structure of singly hydrated, protonated phospho-tyrosine. International Journal of Mass Spectrometry, 2011, 308, 338-347.	1.5	22
34	Structure of Sodiated Polyglycines. Chemistry - A European Journal, 2012, 18, 4583-4592.	3.3	22
35	Gd(III) Polyaminocarboxylate Chelate:Â Realistic Many-Body Molecular Dynamics Simulations for Molecular Imaging Applications. Journal of Physical Chemistry B, 2006, 110, 12848-12851.	2.6	21
36	Assessment of density functionals for predicting the infrared spectrum of sodiated octa-glycine. International Journal of Mass Spectrometry, 2010, 297, 152-161.	1.5	21

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37	Ultraviolet degradation of procymidone â€“ structural characterization by gas chromatography coupled with mass spectrometry and potential toxicity of photoproducts using in silico tests. Rapid Communications in Mass Spectrometry, 2013, 27, 1505-1516.	1.5	21
38	Ultrasoft pseudopotentials for lanthanide solvation complexes: Core or valence character of the 4f electrons. Journal of Chemical Physics, 2006, 124, 164103.	3.0	19
39	Vibrational mode assignment of finite temperature infrared spectra using the AMOEBA polarizable force field. Physical Chemistry Chemical Physics, 2015, 17, 25968-25977.	2.8	19
40	In silico prediction of atomic static electric-dipole polarizabilities of the early tetravalent actinide ions:Th4+(5f0),Pa4+(5f1), andU4+(5f2). Physical Review A, 2008, 78, .	2.5	16
41	Towards energy decomposition analysis for open and closed shell f-elements mono aqua complexes. Chemical Physics Letters, 2013, 563, 25-29.	2.6	16
42	Small molecule activation with divalent samarium triflate: a synergistic effort to cleave O₂. Dalton Transactions, 2018, 47, 9226-9230.	3.3	16
43	Electronic Spectrum of Tryptophan-Phenylalanine. A Correlated Ab Initio and Time-Dependent Density Functional Theory Study. Journal of Physical Chemistry B, 2009, 113, 16443-16448.	2.6	15
44	Electronic Structures of Monoâ€Oxidized Copper and Nickel Phosphasalen Complexes. Chemistry - A European Journal, 2017, 23, 17940-17953.	3.3	15
45	Stepwise Hydration of 2-Aminooxazole: Theoretical Insight into the Structure, Finite Temperature Behavior and Proton-Induced Charge Transfer. Journal of Physical Chemistry A, 2016, 120, 2380-2389.	2.5	14
46	On the accuracy of population analyses based on fitted densities#. Journal of Molecular Modeling, 2017, 23, 99.	1.8	14
47	Structural, energetic and dynamical properties of sodiated oligoglycines: relevance of a polarizable force field. Physical Chemistry Chemical Physics, 2010, 12, 3450.	2.8	13
48	Interactions within the alcohol dehydrogenase Zn(II)â€metalloenzyme active site: Interplay between subvalence, electron correlation/dispersion, and charge transfer/induction effects. International Journal of Quantum Chemistry, 2011, 111, 1213-1221.	2.0	13
49	UV-visible degradation of boscalid - structural characterization of photoproducts and potential toxicity usingin silicotests. Rapid Communications in Mass Spectrometry, 2014, 28, 1153-1163.	1.5	13
50	Theoretical insight into the coordination number of hydrated $$mathrm{Zn}^{2+}$$ Zn 2 + from gas phase to solution. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	13
51	Hydration of the sulfate dianion in size-selected water clusters: From SO42â^'(H2O)9 to SO42â^'(H2O)13. International Journal of Mass Spectrometry, 2017, 418, 15-23.	1.5	13
52	Hydration of the sulfate dianion in cold nanodroplets: SO₄^{2â^'}(H₂O)₁₂and SO₄^{2â^'}(H₂O)₁₃. Physical Chemistry Chemical Physics, 2015, 17, 25935-25945.	2.8	12
53	Structure and Thermodynamics of Mg:Phosphate Interactions in Water: A Simulation Study. ChemPhysChem, 2015, 16, 658-665.	2.1	12
54	Dynamics of ions in a water drop using the AMOEBA polarizable force field. Chemical Physics Letters, 2017, 671, 131-137.	2.6	11

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55	Accuracy of density functionals in the description of dispersion interactions and IR spectra of phosphates and phosphorylated compounds. Journal of Molecular Modeling, 2014, 20, 2426.	1.8	9
56	Bisâ€Cyclooctatetraenyl Thulium(II): Highly Reducing Lanthanide Sandwich Singleâ€Molecule Magnets. Angewandte Chemie, 2021, 133, 6107-6111.	2.0	9
57	Theoretical study of the bent U(Î·8-C8H8)2(CN)â^' complex. Theoretical Chemistry Accounts, 2011, 129, 447-452.	1.4	8
58	Electron transfer in tetramethylbiphosphinine complexes of Cp*₂Yb and Cp*₂Sm. New Journal of Chemistry, 2016, 40, 6643-6649.	2.8	8
59	Reliability and performances of real-time time-dependent auxiliary density functional theory. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	8
60	Divalent Thulium Triflate: A Structural and Spectroscopic Study. Angewandte Chemie, 2017, 129, 4330-4335.	2.0	7
61	Strategy for Modeling the Infrared Spectra of Ion-Containing Water Drops. Journal of Physical Chemistry A, 2018, 122, 832-842.	2.5	7
62	The shape of gaseous nâ€butylbenzene: Assessment of computational methods and comparison with experiments. Journal of Computational Chemistry, 2011, 32, 1550-1560.	3.3	6
63	Reversible electron transfer in organolanthanide chemistry. , 2019, 3, 1.		6
64	Relationship between Conformational Dynamics and Electron Transfer in a Desolvated Peptide. Part I. Structures. Journal of Physical Chemistry B, 2013, 117, 1746-1755.	2.6	5
65	AMOEBA Polarizable Force Field Parameters of the Heme Cofactor in Its Ferrous and Ferric Forms. Journal of Chemical Theory and Computation, 2018, 14, 2705-2720.	5.3	5
66	Infrared Spectra of Deprotonated Dicarboxylic Acids: IRMPD Spectroscopy and Empirical Valenceâ€Bond Modeling. ChemPhysChem, 2019, 20, 803-814.	2.1	5
67	Understanding the structure and electronic properties of Th⁴⁺-water complexes. Canadian Journal of Chemistry, 2013, 91, 821-831.	1.1	4
68	Probing the structural properties of the water solvation shell around gold nanoparticles: A computational study. Journal of Chemical Physics, 2021, 154, 044706.	3.0	4
69	Relationship between Conformational Dynamics and Electron Transfer in a Desolvated Peptide. Part II. Temperature Dependence. Journal of Physical Chemistry B, 2013, 117, 1756-1769.	2.6	3
70	Preventing iron(ii) precipitation in aqueous systems using polyacrylic acid: some molecular insights. Physical Chemistry Chemical Physics, 2018, 20, 18056-18065.	2.8	3
71	Interaction between organic molecules and a gold nanoparticle: a quantum chemical topological analysis. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	3
72	Vibrational spectroscopy of deprotonated peptides containing an acidic side chain. International Journal of Mass Spectrometry, 2019, 435, 42-50.	1.5	2

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73	Atom economical coupling of benzophenone and N-heterocyclic aromatics with SmI₂. Chemical Communications, 2020, 56, 11875-11878.	4.1	2
74	Consistent Picture of Phosphateâ€“Divalent Cation Binding from Models with Implicit and Explicit Electronic Polarization. Journal of Physical Chemistry B, 0, , .	2.6	1
75	RÃ¼cktitelbild: Divalent Thulium Triflate: A Structural and Spectroscopic Study (Angew. Chem. 15/2017). Angewandte Chemie, 2017, 129, 4428-4428.	2.0	0
76	Manifolds of low energy structures for a magic number of hydrated sulfate: SO42â^'(H2O)24. Physical Chemistry Chemical Physics, 2021, 23, 24428-24438.	2.8	0