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	Bisâ€Cyclooctatetraenyl Thulium(II): Highly Reducing Lanthanide Sandwich Singleâ€Molecule Magnets. Angewandte Chemie - International Edition, 2021, 60, 6042-6046.	13.8	27
2	Bisâ€Cyclooctatetraenyl Thulium(II): Highly Reducing Lanthanide Sandwich Singleâ€Molecule Magnets. Angewandte Chemie, 2021, 133, 6107-6111.	2.0	9
3	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
4	Interaction between organic molecules and a gold nanoparticle: a quantum chemical topological analysis. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	3
5	Reliability and performances of real-time time-dependent auxiliary density functional theory. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	8
6	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
7	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
8	Atom economical coupling of benzophenone and N-heterocyclic aromatics with SmI₂. Chemical Communications, 2020, 56, 11875-11878.	4.1	2
9	Infrared Spectra of Deprotonated Dicarboxylic Acids: IRMPD Spectroscopy and Empirical Valenceâ€Bond Modeling. ChemPhysChem, 2019, 20, 803-814.	2.1	5
10	Vibrational spectroscopy of deprotonated peptides containing an acidic side chain. International Journal of Mass Spectrometry, 2019, 435, 42-50.	1.5	2
11	Reversible electron transfer in organolanthanide chemistry. , 2019, 3, 1.		6
12	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
13	Strategy for Modeling the Infrared Spectra of Ion-Containing Water Drops. Journal of Physical Chemistry A, 2018, 122, 832-842.	2.5	7
14	Lanthanidocenes: Synthesis, Structure, and Bonding of Linear Sandwich Complexes of Lanthanides. Journal of the American Chemical Society, 2018, 140, 14433-14439.	13.7	50
15	Small molecule activation with divalent samarium triflate: a synergistic effort to cleave O₂. Dalton Transactions, 2018, 47, 9226-9230.	3.3	16
16	Preventing iron(ii) precipitation in aqueous systems using polyacrylic acid: some molecular insights. Physical Chemistry Chemical Physics, 2018, 20, 18056-18065.	2.8	3
17	Dynamics of ions in a water drop using the AMOEBA polarizable force field. Chemical Physics Letters, 2017, 671, 131-137.	2.6	11
18	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

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19	Divalent Thulium Triflate: A Structural and Spectroscopic Study. Angewandte Chemie - International Edition, 2017, 56, 4266-4271.	13.8	24
20	On the accuracy of population analyses based on fitted densities#. Journal of Molecular Modeling, 2017, 23, 99.	1.8	14
21	RÃ¼cktitelbild: Divalent Thulium Triflate: A Structural and Spectroscopic Study (Angew. Chem. 15/2017). Angewandte Chemie, 2017, 129, 4428-4428.	2.0	0
22	Divalent Thulium Triflate: A Structural and Spectroscopic Study. Angewandte Chemie, 2017, 129, 4330-4335.	2.0	7
23	Electronic Structures of Monoâ€Oxidized Copper and Nickel Phosphasalen Complexes. Chemistry - A European Journal, 2017, 23, 17940-17953.	3.3	15
24	Reductive Disproportionation of CO₂ with Bulky Divalent Samarium Complexes. Organometallics, 2017, 36, 4660-4668.	2.3	30
25	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
26	Assessment of Density Functionals for Computing Thermodynamic Properties of Lanthanide Complexes. ChemPhysChem, 2017, 18, 2688-2696.	2.1	25
27	Simulating Electron Dynamics in Polarizable Environments. Journal of Chemical Theory and Computation, 2017, 13, 3985-4002.	5.3	41
28	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
29	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
30	Electron transfer in tetramethylbiphosphinine complexes of Cp*₂Yb and Cp*₂Sm. New Journal of Chemistry, 2016, 40, 6643-6649.	2.8	8
31	Chirality-dependent structuration of protonated or sodiated polyphenylalanines: IRMPD and ion mobility studies. Physical Chemistry Chemical Physics, 2016, 18, 1807-1817.	2.8	27
32	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
33	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
34	Structure and Thermodynamics of Mg:Phosphate Interactions in Water: A Simulation Study. ChemPhysChem, 2015, 16, 658-665.	2.1	12
35	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
36	Finite Temperature Infrared Spectra from Polarizable Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 3190-3199.	5.3	23

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37	Multiple One-Electron Transfers in Bipyridine Complexes of Bis(phospholyl) Thulium. Organometallics, 2014, 33, 4100-4106.	2.3	31
38	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
39	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
40	Theoretical Insights into the Nature of Divalent Lanthanideâ€“Ligand Interactions. Organometallics, 2013, 32, 1265-1271.	2.3	34
41	Understanding the structure and electronic properties of Th⁴⁺-water complexes. Canadian Journal of Chemistry, 2013, 91, 821-831.	1.1	4
42	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
43	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
44	Towards energy decomposition analysis for open and closed shell f-elements mono aqua complexes. Chemical Physics Letters, 2013, 563, 25-29.	2.6	16
45	Ab Initio Extension of the AMOEBA Polarizable Force Field to Fe²⁺. Journal of Chemical Theory and Computation, 2013, 9, 3062-3071.	5.3	31
46	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
47	Globule to Helix Transition in Sodiated Polyalanines. Journal of Physical Chemistry Letters, 2012, 3, 3320-3324.	4.6	33
48	A new, centered 32-electron system: the predicted [U@Si20]6â^'-like isoelectronic series. Chemical Science, 2012, 3, 2843.	7.4	42
49	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
50	Structure of Sodiated Polyglycines. Chemistry - A European Journal, 2012, 18, 4583-4592.	3.3	22
51	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
52	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
53	Structure of singly hydrated, protonated phospho-tyrosine. International Journal of Mass Spectrometry, 2011, 308, 338-347.	1.5	22
54	Theoretical study of the bent U(Î·8-C8H8)2(CN)â^' complex. Theoretical Chemistry Accounts, 2011, 129, 447-452.	1.4	8

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55	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
56	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
57	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
58	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
59	Chemical properties of the predicted 32-electron systems Pu@Sn12 and Pu@Pb12. Comptes Rendus Chimie, 2010, 13, 884-888.	0.5	26
60	Structural, energetic and dynamical properties of sodiated oligoglycines: relevance of a polarizable force field. Physical Chemistry Chemical Physics, 2010, 12, 3450.	2.8	13
61	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
62	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
63	IRMPD Spectroscopy of a Protonated, Phosphorylated Dipeptide. ChemPhysChem, 2008, 9, 2564-2573.	2.1	33
64	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
65	Towards a 32-Electron Principle: Pu@Pb12 and Related Systems. Angewandte Chemie - International Edition, 2007, 46, 1427-1430.	13.8	88
66	Ultrasoft pseudopotentials for lanthanide solvation complexes: Core or valence character of the 4f electrons. Journal of Chemical Physics, 2006, 124, 164103.	3.0	19
67	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
68	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
69	Theoretical study of the hydrated Gd3+ ion: Structure, dynamics, and charge transfer. Journal of Chemical Physics, 2006, 124, 074505.	3.0	56
70	Accurate static electric dipole polarizability calculations of +3 charged lanthanide ions. Chemical Physics, 2005, 311, 169-176.	1.9	32
71	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
72	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

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73	Calculation of harmonic and anharmonic vibrational wavenumbers for triatomic uranium compounds XUY. Chemical Physics, 2004, 302, 1-11.	1.9	36
74	Modeling of Uranyl Cationâ^'Water Clusters. Journal of Physical Chemistry B, 2003, 107, 3051-3060.	2.6	76
75	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
76	Consistent Picture of Phosphateâ€“Divalent Cation Binding from Models with Implicit and Explicit Electronic Polarization. Journal of Physical Chemistry B, 0, , .	2.6	1