Aurora Clark

List of Publications by Year
in descending order

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121 papers	3,003 citations	159358 30 h-index	189595 50 g-index
134 all docs	134 docs citations	134 times ranked	3421 citing authors

#	Article	IF	Citations
1	Local spin. Journal of Chemical Physics, 2001, 115, 7382-7392.	1.2	165
2	Beyond Exciton Theory:â€‰ A Time-Dependent DFT and Franckâ˜Condon Study of Perylene Diimide and Its Chromophoric Dimer. Journal of the American Chemical Society, 2007, 129, 7586-7595.	6.6	148
3	DFT characterization of the optical and redox properties of natural pigments relevant to dye-sensitized solar cells. Chemical Physics Letters, 2007, 438, 26-30.	1.2	147
4	Mechanisms of Water Oxidation Catalyzed by Ruthenium Diimine Complexes. Inorganic Chemistry, 2008, 47, 1753-1764.	1.9	119
5	Density and wave function analysis of actinide complexes: What can fuzzy atom, atoms-in-molecules, Mulliken, Loîwdin, and natural population analysis tell us?. Journal of Chemical Physics, 2004, 121, 2563.	1.2	97
6	ChemNetworks: A complex network analysis tool for chemical systems. Journal of Computational Chemistry, 2014, 35, 495-505.	1.5	83
7	MoleculaRnetworks: An integrated graph theoretic and data mining tool to explore solvent organization in molecular simulation. Journal of Computational Chemistry, 2012, 33, 853-860.	1.5	81
8	Local spin II. Molecular Physics, 2002, 100, 373-383.	0.8	76
9	Population analyses that utilize projection operators. International Journal of Quantum Chemistry, 2003, 93, 384-394.	1.0	70
10	UDFT and MCSCF Descriptions of the Photochemical Bergman Cyclization of Enediynes. Journal of the American Chemical Society, 2001, 123, 2650-2657.	6.6	67
11	Structural and Dielectric Properties of Quartzâ˜Water Interfaces. Journal of Physical Chemistry C, 2008, 112, 19986-19994.	1.5	67
12	A Phenyliodonium Ylide as a Precursor for Dicarboethoxycarbene:Â Demonstration of a Strategy for Carbene Generation. Journal of the American Chemical Society, 2000, 122, 5210-5211.	6.6	66
13	Trends in Aqueous Hydration Across the 4f Period Assessed by Reliable Computational Methods. Inorganic Chemistry, 2010, 49, 7808-7817.	1.9	66
14	LÃ¶wdin population analysis with and without rotational invariance. International Journal of Quantum Chemistry, 2006, 106, 2065-2072.	1.0	65
15	Hydration Properties of Aqueous Pb(II) Ion. Inorganic Chemistry, 2008, 47, 8233-8241.	1.9	65
16	Density Functional and Basis Set Dependence of Hydrated Ln(III) Properties. Journal of Chemical Theory and Computation, 2008, 4, 708-718.	2.3	53
17	Local Spin III:Â Wave Function Analysis along a Reaction Coordinate, H Atom Abstraction, and Addition Processes of Benzyne. Journal of Physical Chemistry A, 2002, 106, 6890-6896.	1.1	52
18	Analysis of wave functions for open-shell molecules. Physical Chemistry Chemical Physics, 2007, 9, 1881.	1.3	52

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19	Deconstructing Hydrogen-Bond Networks in Confined Nanoporous Materials: Implications for Alcoholâ€“Water Separation. Journal of Physical Chemistry C, 2014, 118, 19723-19732.	1.5	50
20	Photothermally Induced Bergman Cyclization of Metalloenediynes via Near-Infrared Ligand-to-Metal Charge-Transfer Excitation. Inorganic Chemistry, 2003, 42, 1663-1672.	1.9	48
21	ForceFit: A code to fit classical force fields to quantum mechanical potential energy surfaces. Journal of Computational Chemistry, 2010, 31, 2307-2316.	1.5	48
22	Spin polarization and annihilation for radicals and diradicals. International Journal of Quantum Chemistry, 2005, 103, 1-9.	1.0	44
23	Thermodynamic and Structural Features of Aqueous Ce(III). Journal of Physical Chemistry A, 2008, 112, 11198-11206.	1.1	43
24	Time-Dependent Density Functional Theory Studies of the Photoswitching of the Two-Photon Absorption Spectra in Stilbene, Metacyclophenadiene, and Diarylethene Chromophores. Journal of Physical Chemistry A, 2006, 110, 3790-3796.	1.1	42
25	Electronic Structure, Excited States, and Photoelectron Spectra of Uranium, Thorium, and Zirconium Bis(Ketimido) Complexes (C5R5)2M[â^'NCPh2]2(M = Th, U, Zr; R = H, CH3). Journal of Physical Chemistry A, 2005, 109, 5481-5491.	1.1	40
26	Titanium(IV) Trifluoromethyl Complexes: New Perspectives on Bonding from Organometallic Fluorocarbon Chemistry. Organometallics, 2012, 31, 1484-1499.	1.1	37
27	Model Studies of Hydrogen Atom Addition and Abstraction Processes Involving ortho-, meta-, and para-Benzynes. Journal of the American Chemical Society, 2001, 123, 10691-10698.	6.6	35
28	Model Molecular Magnets. Journal of Physical Chemistry A, 2002, 106, 7456-7461.	1.1	34
29	Ab Initio Molecular Dynamics Reveal Spectroscopic Siblings and Ion Pairing as New Challenges for Elucidating Prenucleation Aluminum Speciation. Journal of Physical Chemistry B, 2018, 122, 7394-7402.	1.2	34
30	In Situ ²⁷Al NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions above and below Saturation with Respect to Gibbsite. Inorganic Chemistry, 2018, 57, 11864-11873.	1.9	33
31	Structure and Dynamics of NaCl Ion Pairing in Solutions of Water and Methanol. Journal of Physical Chemistry B, 2015, 119, 15652-15661.	1.2	31
32	Surfactant-enhanced heterogeneity of the aqueous interface drives water extraction into organic solvents. Physical Chemistry Chemical Physics, 2019, 21, 2866-2874.	1.3	31
33	Towards a unified description of the hydrogen bond network of liquid water: A dynamics based approach. Journal of Chemical Physics, 2014, 141, 214107.	1.2	30
34	Ligand Substituent Effect Observed for Ytterbocene 4â€˜-Cyano-2,2â€˜:6â€˜,2â€˜Ââ€˜-terpyridine. Inorganic Chemistry, 2005, 44, 5911-5920.	1.9	29
35	An Assessment of Computational Methods for Obtaining Structural Information of Moderately Flexible Biomolecules from Ion Mobility Spectrometry. Journal of the American Society for Mass Spectrometry, 2012, 23, 792-805.	1.2	29
36	Heavy Anionic Complex Creates a Unique Water Structure at a Soft Charged Interface. Journal of Physical Chemistry C, 2018, 122, 29228-29236.	1.5	29

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37	p-Benzyne Derivatives That Have Exceptionally Small Singletâ^'Triplet Gaps and Even a Triplet Ground State. Journal of Organic Chemistry, 2003, 68, 3387-3396.	1.7	27
38	Deconstructing the Confinement Effect upon the Organization and Dynamics of Water in Hydrophobic Nanoporous Materials: Lessons Learned from Zeolites. Journal of Physical Chemistry C, 2017, 121, 22015-22024.	1.5	27
39	Origins of Clustering of Metalateâ€"Extractant Complexes in Liquidâ€"Liquid Extraction. ACS Applied Materials & Interfaces, 2021, 13, 24194-24206.	4.0	27
40	Integrated Computational and Experimental Protocol for Understanding Rh(III) Speciation in Hydrochloric and Nitric Acid Solutions. Inorganic Chemistry, 2014, 53, 12315-12322.	1.9	23
41	Novel Analysis of Cation Solvation Using a Graph Theoretic Approach. Journal of Physical Chemistry B, 2012, 116, 4263-4275.	1.2	21
42	Isolation of electronic from geometric contributions to Bergman cyclization of metalloenediynesElectronic supplementary information (ESI) available: syntheses, characterizations and DSC traces of 1â€"3, crystallographic data of 1â€"4. See http://www.rsc.org/suppdata/cc/b3/b301690k/. Chemical Communications, 2003, , 1156-1157.	2.2	20
43	Determining polyhedral arrangements of atoms using PageRank. Journal of Mathematical Chemistry, 2012, 50, 2342-2350.	0.7	19
44	Solutes at the liquid:liquid phase boundaryâ€"Solubility and solvent conformational response alter interfacial microsolvation. Journal of Chemical Physics, 2015, 142, 104707.	1.2	17
45	Preferential Solvation of Metastable Phases Relevant to Topological Control Within the Synthesis of Metalâ€"Organic Frameworks. Inorganic Chemistry, 2014, 53, 8930-8940.	1.9	16
46	Determining the water content of a drift gas using reduced ion mobility measurements. International Journal of Mass Spectrometry, 2014, 368, 37-44.	0.7	16
47	Sensitivity of Solvation Environment to Oxidation State and Position in the Early Actinide Period. Inorganic Chemistry, 2015, 54, 6216-6225.	1.9	16
48	Applications of Polarizable Continuum Models To Determine Accurate Solution-Phase Thermochemical Values Across a Broad Range of Cation Charge â€" The Case of U(IIIâ€"VI). Journal of Chemical Theory and Computation, 2015, 11, 55-63.	2.3	16
49	The Middle Science: Traversing Scale In Complex Many-Body Systems. ACS Central Science, 2021, 7, 1271-1287.	5.3	16
50	Dynamics of Interfacial Electron Transfer from Betanin to Nanocrystalline TiO₂: The Pursuit of Two-Electron Injection. Journal of Physical Chemistry C, 2015, 119, 19030-19041.	1.5	15
51	²⁷Al Pulsed Field Gradient, Diffusionâ€"NMR Spectroscopy of Solvation Dynamics and Ion Pairing in Alkaline Aluminate Solutions. Journal of Physical Chemistry B, 2018, 122, 10907-10912.	1.2	15
52	Trends in Ln(III) Sorption to Quartz Assessed by Molecular Dynamics Simulations and Laser-Induced Fluorescence Studies. Journal of Physical Chemistry C, 2011, 115, 21120-21127.	1.5	14
53	Intermolecular network analysis of the liquid and vapor interfaces of pentane and water: microsolvation does not trend with interfacial properties. Physical Chemistry Chemical Physics, 2014, 16, 12475-12487.	1.3	14
54	Resolving local configurational contributions to X-ray and neutron radial distribution functions within solutions of concentrated electrolytes â€" a case study of concentrated NaOH. Physical Chemistry Chemical Physics, 2019, 21, 6828-6838.	1.3	14

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55	Structural and Thermodynamic Properties of the Cm^{III} Ion Solvated by Water and Methanol. Inorganic Chemistry, 2016, 55, 4992-4999.	1.9	13
56	Influence of aqueous ionic strength upon liquid:liquid interfacial structure and microsolvation. Fluid Phase Equilibria, 2016, 407, 126-134.	1.4	13
57	Xâ€ray absorption signatures of hydrogenâ€bond structure in waterâ€“alcohol solutions. International Journal of Quantum Chemistry, 2019, 119, e25802.	1.0	13
58	Competitive Interactions at Electrolyte/Octanol Interfaces: A Molecular Perspective. Journal of Physical Chemistry C, 2020, 124, 10924-10934.	1.5	13
59	Amphiphile Organization in Organic Solutions: An Alternative Explanation for Small-Angle X-ray Scattering Features in Malonamide/Alkane Mixtures. Journal of Physical Chemistry B, 2020, 124, 10822-10831.	1.2	13
60	Water Organization and Dynamics on Mineral Surfaces Interrogated by Graph Theoretical Analyses of Intermolecular Chemical Networks. Minerals (Basel, Switzerland), 2014, 4, 118-129.	0.8	12
61	Coupled Multimodal Dynamics of Hydrogen-Containing Ion Networks in Water-Deficient, Sodium Hydroxide-Aluminate Solutions. Journal of Physical Chemistry B, 2018, 122, 12097-12106.	1.2	12
62	Square supramolecular assemblies of uranyl complexes in organic solvents. Chemical Communications, 2018, 54, 10064-10067.	2.2	12
63	Amphiphile-Based Complex Fluids: The Self-Assembly Ensemble as Protagonist. ACS Central Science, 2019, 5, 10-12.	5.3	12
64	Solid-State Recrystallization Pathways of Sodium Aluminate Hydroxy Hydrates. Inorganic Chemistry, 2020, 59, 6857-6865.	1.9	11
65	Hierarchical phenomena in multicomponent liquids: simulation methods, analysis, chemistry. Physical Chemistry Chemical Physics, 2020, 22, 9850-9874.	1.3	11
66	The role of basis set superposition error in water addition reactions to Ln(III) cations. International Journal of Quantum Chemistry, 2009, 109, 2474-2481.	1.0	10
67	Structure Modulated Electronic Contributions to Metalloenediyne Reactivity: Synthesis and Thermal Bergman Cyclization of MLX2 Compounds. Inorganic Chemistry, 2009, 48, 3916-3925.	1.9	10
68	Influence of bidentate ligand donor types on the formation and stability in 2 + 1 fac-[M^I(CO)₃]⁺ (M = Re, ^{99m}Tc) complexes. Dalton Transactions, 2017, 46, 1134-1144.	1.6	10
69	Structural and Dynamic Heterogeneity of Capillary Wave Fronts at Aqueous Interfaces. Journal of Physical Chemistry B, 2017, 121, 9052-9062.	1.2	10
70	Effect of Ions on the Optical Absorption Spectra of Aqueously Solvated Chromophores. Journal of Physical Chemistry A, 2019, 123, 6175-6184.	1.1	10
71	PageRank as a collective variable to study complex chemical transformations and their energy landscapes. Journal of Chemical Physics, 2019, 150, 134102.	1.2	10
72	Inference of principal species in caustic aluminate solutions through solid-state spectroscopic characterization. Dalton Transactions, 2020, 49, 5869-5880.	1.6	10

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73	â€œCovalent Hydrationâ€•Reactions in Model Monomeric Ru 2,2â€²-Bipyridine Complexes: Thermodynamic Favorability as a Function of Metal Oxidation and Overall Spin States. Inorganic Chemistry, 2011, 50, 8177-8187.	1.9	9
74	A Combined Density Functional Theory and Spectrophotometry Study of the Bonding Interactions of [NpO₂Â·M]⁴⁺ Cationâ€“Cation Complexes. Inorganic Chemistry, 2017, 56, 4788-4795.	1.9	9
75	Anticorrelated Contributions to Pre-edge Features of Aluminate Near-Edge X-ray Absorption Spectroscopy in Concentrated Electrolytes. Journal of Physical Chemistry Letters, 2018, 9, 2444-2449.	2.1	9
76	Representations of energy landscapes by sublevelset persistent homology: An example with n-alkanes. Journal of Chemical Physics, 2021, 154, 114114.	1.2	9
77	Shear stress dependence of force networks in 3D dense suspensions. Soft Matter, 2021, 17, 7476-7486.	1.2	9
78	Density Functional Analysis of Ancillary Ligand Electronic Contributions to Metal-Mediated Enediyne Cyclization. Inorganic Chemistry, 2009, 48, 3926-3933.	1.9	8
79	Sensitivity of the properties of ruthenium â€œblue dimerâ€•to method, basis set, and continuum model. Journal of Chemical Physics, 2012, 136, 204104.	1.2	8
80	Coupled-cluster, MÃ¶ller Plesset (MP2), density fitted local MP2, and density functional theory examination of the energetic and structural features of hydrophobic solvation: Water and pentane. Journal of Chemical Physics, 2012, 136, 054305.	1.2	8
81	A homoleptic chromium(<scp>iii</scp>) carboxylate. Dalton Transactions, 2018, 47, 4790-4793.	1.6	8
82	Global topology of contact force networks: Insight into shear thickening suspensions. Physical Review E, 2019, 99, 012607.	0.8	8
83	Mechanisms of Al³⁺ Dimerization in Alkaline Solutions. Inorganic Chemistry, 2020, 59, 18181-18189.	1.9	8
84	The â€œHoleâ€•Story in Ionized Water from the Perspective of Ehrenfest Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 9946-9951.	2.1	8
85	Ferrous Iron Reduction of Superoxide, A Proton-Coupled Electron-Transfer Four-Point Test. Journal of Physical Chemistry A, 2009, 113, 1020-1025.	1.1	7
86	Intermolecular Network Theory. Annual Reports in Computational Chemistry, 2015, 11, 313-359.	0.9	7
87	Competitive Interactions Within Cm(III) Solvation in Binary Water/Methanol Solutions. Inorganic Chemistry, 2018, 57, 10050-10058.	1.9	7
88	The role of surfactant force field on the properties of liquid/liquid interfaces. Fluid Phase Equilibria, 2020, 511, 112497.	1.4	7
89	Correlation between Rheological Properties of Zinc Carboxylate Liquids and Molecular Structure. Journal of Physical Chemistry B, 2007, 111, 7073-7077.	1.2	6
90	Building Self-Assembled Molecular Layers with Axially Substituted Titanium Phthalocyanines. Langmuir, 2010, 26, 12709-12715.	1.6	6

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91	The surface structure of Î±-uranophane and its interaction with Eu(III) â€“ An integrated computational and fluorescence spectroscopy study. Geochimica Et Cosmochimica Acta, 2013, 103, 184-196.	1.6	6
92	Rh(III) Extraction by Phosphinic Acids from Nitrate Media. Solvent Extraction and Ion Exchange, 2015, 33, 418-428.	0.8	6
93	The Role of Excited-State Proton Relays in the Photochemical Dynamics of Water Nanodroplets. Journal of Physical Chemistry Letters, 2019, 10, 3694-3698.	2.1	6
94	Cluster Identification Using Modularity Optimization to Uncover Chemical Heterogeneity in Complex Solutions. Journal of Physical Chemistry A, 2021, 125, 3986-3993.	1.1	6
95	Uranyl Speciation in the Presence of Specific Ion Gradients at the Electrolyte/Organic Interface. Solvent Extraction and Ion Exchange, 0, , 1-23.	0.8	6
96	A TDDFT description of the low-energy excited states of copper and zinc metalloenediynesElectronic supplementary information (ESI) available: Cartesian coordinates of optimized structures and tables of the TDDFT configurations for each excited state. See http://www.rsc.org/suppdata/cc/b3/b308633j/. Chemical Communications, 2003, , 2876.	2.2	5
97	A viewpoint on population analyses. International Journal of Quantum Chemistry, 2022, 122, .	1.0	5
98	Molecular dynamics and network analysis reveal the contrasting roles of polar solutes within organic phase amphiphile aggregation. Journal of Molecular Liquids, 2022, 359, 119226.	2.3	5
99	Static electric dipole polarizabilities of An5+/6+ and AnO2+/2+ (An = U, Np, and Pu) ions. Journal of Chemical Physics, 2014, 141, 234304.	1.2	4
100	Efficient Intermolecular Energy Exchange and Soft Ionization of Water at Nanoplatelet Interfaces. Journal of Physical Chemistry Letters, 2020, 11, 10088-10093.	2.1	4
101	An octanol hinge opens the door to water transport. Chemical Science, 2021, 12, 2294-2303.	3.7	4
102	Theory-Guided Inelastic Neutron Scattering of Crystalline Alkaline Aluminate Salts Bearing Principal Motifs of Solution-State Species. Inorganic Chemistry, 2021, 60, 16223-16232.	1.9	4
103	pH dependent reactivity of boehmite surfaces from first principles molecular dynamics. Physical Chemistry Chemical Physics, 2022, 24, 14177-14186.	1.3	4
104	Static Electric Dipole Polarizabilities of Tri- and Tetravalent U, Np, and Pu Ions. Journal of Physical Chemistry A, 2013, 117, 11874-11880.	1.1	3
105	H2 Adsorbed Site-to-Site Electronic Delocalization within IRMOF-1: Understanding Non-Negligible Interactions at High Pressure. Materials, 2016, 9, 578.	1.3	3
106	Acceleration of metalâ€“ligand complexation kinetics by electrospray ionization. Analyst, The, 2017, 142, 4468-4475.	1.7	3
107	A Geometric Measure Theory Approach to Identify Complex Structural Features on Soft Matter Surfaces. Journal of Chemical Theory and Computation, 2020, 16, 4579-4587.	2.3	3
108	Al27 NMR chemical shift of Al(OH)4â˜ calculated from first principles: Assessment of error cancellation in chemically distinct reference and target systems. Journal of Chemical Physics, 2020, 152, 134303.	1.2	3

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109	Essential Aspects of Solvent Effects and Solution Conditions upon the Modeling and Simulation of Lanthanide and Actinide Complexes. ACS Symposium Series, 0, , 249-276.	0.5	3
110	Alcohol Clustering Mechanisms in Supercritical Carbon Dioxide Using Pulsed-Field Gradient, Diffusion NMR and Network Analysis: Feedback on Stepwise Self-Association Models. Journal of Physical Chemistry B, 2019, 123, 5316-5323.	1.2	2
111	Unexpected inverse correlations and cooperativity in ion-pair phase transfer. Chemical Science, 2021, 12, 13930-13939.	3.7	2
112	Persistent Homology Metrics Reveal Quantum Fluctuations and Reactive Atoms in Path Integral Dynamics. Frontiers in Chemistry, 2021, 9, 624937.	1.8	2
113	Behavior of Linear and Nonlinear Dimensionality Reduction for Collective Variable Identification of Small Molecule Solution-Phase Reactions. Journal of Chemical Theory and Computation, 2022, 18, 1286-1296.	2.3	2
114	Radiochemistry Education at Washington State University: Sustaining Academic Radiochemistry for the Nation. , 2009, , .		1
115	Modulation of hydride formation energies in transition metal doped Mg by alteration of spin state. Chemical Physics Letters, 2013, 560, 10-14.	1.2	1
116	Rethinking the magnetic properties of lepidocrocite: A density functional theory and cluster expansion study. Journal of Applied Physics, 2020, 128, .	1.1	1
117	Ensemble effects on allylic oxidation within explicit solvation environments. Dalton Transactions, 2021, 50, 9259-9268.	1.6	1
118	p-Benzyne Derivatives that Have Exceptionally Small Singletâ€"Triplet Gaps and Even a Triplet Ground State.. ChemInform, 2003, 34, no.	0.1	0
119	Gradient fit functions for two-body potential energy surfaces based upon a harmonic series. Molecular Simulation, 2010, 36, 335-340.	0.9	0
120	DELTA-Topology: A Science Gateway for Experimental and Computational Chemical Data Analysis using Topological Models. , 2021, , .		0
121	Special Issue on Hierarchical Organization in Solvent Extraction. Solvent Extraction and Ion Exchange, 2022, 40, 1-5.	0.8	0