Alain Chaumont

List of Publications by Citations

66 papers	1,653 citations	22 h-index	39 g-index
67 ext. papers	1,770 ext. citations	4.7 avg, IF	4.75 L-index

#	Paper	IF	Citations
66	Ab initio molecular dynamics of liquid 1,3-dimethylimidazolium chloride. *Journal of Physical Chemistry B*, **2005**, 109, 18591-9	3.4	188
65	Aqueous interfaces with hydrophobic room-temperature ionic liquids: a molecular dynamics study. *Journal of Physical Chemistry B*, **2005**, 109, 18964-73	3.4	123
64	Solvation of uranyl(II) and europium(III) cations and their chloro complexes in a room-temperature ionic liquid. A theoretical study of the effect of solvent "humidity". *Inorganic Chemistry*, **2004**, 43, 5891-901	5.1	100
63	Solvation of M3+ lanthanide cations in room-temperature ionic liquids. A molecular dynamics investigation. *Physical Chemistry Chemical Physics*, **2003**, 5, 3481-3488	3.6	86
62	Europium(III) and its halides in anhydrous room-temperature imidazolium-based ionic liquids: a combined TRES, EXAFS, and molecular dynamics study. *Inorganic Chemistry*, **2005**, 44, 8355-67	5.1	84
61	Uranyl coordination in ionic liquids: the competition between ionic liquid anions, uranyl counterions, and Cl- anions investigated by extended X-ray absorption fine structure and UV-visible spectroscopies and molecular dynamics simulations. *Inorganic Chemistry*, **2007**, 46, 4815-26	5.1	82
60	Uranyl and strontium salt solvation in room-temperature ionic liquids. A molecular dynamics investigation. *Inorganic Chemistry*, **2003**, 42, 5348-56	5.1	61
59	Ion aggregation in concentrated aqueous and methanol solutions of polyoxometallates Keggin anions: the effect of counterions investigated by molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2008**, 10, 6940-53	3.6	56
58	Solvation of uranyl(II), europium(III) and europium(II) cations in "basic" room-temperature ionic liquids: a theoretical study. *Chemistry - A European Journal*, **2004**, 10, 3919-30	4.8	52
57	M3+ Lanthanide Chloride Complexes in Neutral Room Temperature Ionic Liquids: A Theoretical Study. *Journal of Physical Chemistry B*, **2004**, 108, 3311-3319	3.4	50
56	Water versus acetonitrile coordination to uranyl. Density functional study of cooperative polarization effects in solution. *Inorganic Chemistry*, **2011**, 50, 299-308	5.1	48
55	Cation extraction by 18-crown-6 to a room-temperature ionic liquid: The effect of solvent humidity investigated by molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2005**, 7, 124-135	3.6	38
54	Solvation of Ln((III)) lanthanide cations in the [BMI][SCN], [MeBu(3)N][SCN], and [BMI](5)[Ln(NCS)(8)] ionic liquids: a molecular dynamics study. *Inorganic Chemistry*, **2009**, 48, 4277-89	5.1	37
53	Solvation of fluoro and mixed fluoro/chloro complexes of Eu(III) in the [BMI][PF6] room temperature ionic liquid. A theoretical study. *Physical Chemistry Chemical Physics*, **2005**, 7, 1926-32	3.6	36
52	Competitive complexation of nitrates and chlorides to uranyl in a room temperature ionic liquid. *Inorganic Chemistry*, **2010**, 49, 6484-94	5.1	35
51	Solvation of uranyl-CMPO complexes in dry vs. humid forms of the [BMI][PF6] ionic liquid. A molecular dynamics study. *Physical Chemistry Chemical Physics*, **2006**, 8, 494-502	3.6	34
50	Polyoxometalate Keggin Anions at Aqueous Interfaces with Organic Solvents, Ionic Liquids, and Graphite: a Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2009**, 113, 18233-18243	3.8	32

49	Supported Catalytically Active Supramolecular Hydrogels for Continuous Flow Chemistry. *Angewandte Chemie - International Edition*, **2019**, 58, 18817-18822	16.4	23
48	Water versus acetonitrile coordination to uranyl. Effect of chloride ligands. *Inorganic Chemistry*, **2012**, 51, 1943-52	5.1	23
47	Interactions between Keggin Anions in Water: The Higher Their Charge, the Higher Their Condensation? A Simulation Study. *European Journal of Inorganic Chemistry*, **2013**, 2013, 1835-1853	2.3	23
46	Strontium nitrate extraction to ionic liquids by a crown ether: a molecular dynamics study of aqueous interfaces with C4mim+- vs C8mim+-based ionic liquids. *Journal of Physical Chemistry B*, **2010**, 114, 13773-85	3.4	23
45	Do Keggin anions repulse each other in solution? The effect of solvent, counterions and ion representation investigated by free energy (PMF) simulations. *Comptes Rendus Chimie*, **2012**, 15, 107-117	2.7	22
44	Solvation of Big Spherical solutes in room temperature ionic liquids and at their aqueous interface: A molecular dynamics simulation study. *Journal of Molecular Liquids*, **2007**, 131-132, 36-47	6	22
43	Control of Surface-Localized, Enzyme-Assisted Self-Assembly of Peptides through Catalyzed Oligomerization. *Langmuir*, **2017**, 33, 8267-8276	4	21
42	Halide anion solvation and recognition by a macrotricyclic tetraammonium host in an ionic liquid: a molecular dynamics study. *New Journal of Chemistry*, **2006**, 30, 537	3.6	21
41	Nature of Zr-monosubstituted monomeric and dimeric polyoxometalates in water solution at different pH conditions: static density functional theory calculations and dynamic simulations. *Inorganic Chemistry*, **2014**, 53, 778-86	5.1	20
40	Supramolecular Hydrogel Induced by Electrostatic Interactions between Polycation and Phosphorylated-Fmoc-Tripeptide. *Chemistry of Materials*, **2020**, 32, 1946-1956	9.6	19
39	Perrhenate complexation by uranyl in traditional solvents and in ionic liquids: a joint molecular dynamics/spectroscopic study. *Journal of Physical Chemistry B*, **2012**, 116, 3205-19	3.4	19
38	Macrotricyclic quaternary tetraammonium receptors: halide anion recognition and interfacial activity at an aqueous interface. A molecular dynamics investigation. *Journal of Computational Chemistry*, **2002**, 23, 1532-43	3.5	19
37	Mimicking the Chemistry of Natural Eumelanin Synthesis: The KE Sequence in Polypeptides and in Proteins Allows for a Specific Control of Nanosized Functional Polydopamine Formation. *Biomacromolecules*, **2018**, 19, 3693-3704	6.9	18
36	Autonomous Growth of a Spatially Localized Supramolecular Hydrogel with Autocatalytic Ability. *Angewandte Chemie - International Edition*, **2020**, 59, 14558-14563	16.4	17
35	Importance of the Liquid Liquid Interface in Assisted Ion Extraction: New Molecular Dynamics Studies of Cesium Picrate Extraction by a Calix[4]arene. *Journal of Physical Chemistry C*, **2009**, 113, 10610-10622	3.8	17
34	Unraveling the role of water in the stereoselective step of aqueous proline-catalyzed aldol reactions. *Chemistry - A European Journal*, **2012**, 18, 15868-74	4.8	16
33	Potential proton-release channels in bacteriorhodopsin. *ChemPhysChem*, **2008**, 9, 2751-8	3.2	16
32	Chloride complexation by uranyl in a room temperature ionic liquid. A computational study. *Journal of Physical Chemistry B*, **2008**, 112, 12014-23	3.4	14

31	Titanium oxo-clusters derivatized from the Ti10O12(cat)8(py)8 complex: structural investigation and spectroscopic studies of light absorption. *Dalton Transactions*, **2016**, 45, 8760-9	4.3	14
30	Assembly Mechanism of Zr-Containing and Other TM-Containing Polyoxometalates. *Inorganic Chemistry*, **2017**, 56, 4148-4156	5.1	12
29	Is Charge Scaling Really Mandatory when Developing Fixed-Charge Atomistic Force Fields for Deep Eutectic Solvents?. *Journal of Physical Chemistry B*, **2020**, 124, 7239-7250	3.4	12
28	Monomeric Ti(iv)-based complexes incorporating luminescent nitrogen ligands: synthesis, structural characterization, emission spectroscopy and cytotoxic activities. *Dalton Transactions*, **2016**, 45, 19072-19085	4.3	11
27	Stretch-Induced Helical Conformations in Poly(l-lysine)/Hyaluronic Acid Multilayers. *ACS Applied Materials & Interfaces*, **2016**, 8, 14958-65	9.5	11
26	Halide anion capture and recognition by a tetrahedral tetraammonium receptor in water: a molecular dynamics investigation. *Chemistry - A European Journal*, **2003**, 9, 635-43	4.8	11
25	Speciation of La(III) chloride complexes in water and acetonitrile: a density functional study. *Inorganic Chemistry*, **2012**, 51, 13396-407	5.1	8
24	Accumulation of host–guest ion complexes with different counterions at the water–supercritical CO2 interface: a molecular dynamics study. *Russian Chemical Bulletin*, **2004**, 53, 1459-1465	1.7	7
23	Formation of Long, Multicenter [TCNE] Dimers in Solution: Solvation and Stability Assessed through Molecular Dynamics Simulations. *Chemistry - A European Journal*, **2016**, 22, 17037-17046	4.8	7
22	Distributed polarizability models for imidazolium-based ionic liquids. *Journal of Physical Chemistry A* , **2014**, 118, 8842-51	2.8	6
21	Supported Catalytically Active Supramolecular Hydrogels for Continuous Flow Chemistry. *Angewandte Chemie*, **2019**, 131, 18993-18998	3.6	5
20	A Bis-Acridinium Macrocycle as Multi-Responsive Receptor and Selective Phase-Transfer Agent of Perylene. *Angewandte Chemie - International Edition*, **2020**, 59, 23206-23212	16.4	5
19	Autonomous Growth of a Spatially Localized Supramolecular Hydrogel with Autocatalytic Ability. *Angewandte Chemie*, **2020**, 132, 14666-14671	3.6	4
18	Bromide complexation by the Eu(III) lanthanide cation in dry and humid ionic liquids: a molecular dynamics PMF study. *ChemPhysChem*, **2012**, 13, 1677-86	3.2	4
17	Simulations of the Dynamics of 18-Crown-6 and its Complexes: From the Gas Phase to Aqueous Interfaces with SC-CO2 and a Room-Temperature Ionic Liquid **2005**, 327-348		4
16	Bent 1,10-Phenanthroline Ligands within Octahedral Complexes Constructed around a TiON Core. *Inorganic Chemistry*, **2020**, 59, 12005-12016	5.1	4
15	Dipyrrolyldiketonato Titanium(IV) Complexes from Monomeric to Multinuclear Architectures: Synthesis, Stability, and Liquid-Crystal Properties. *Inorganic Chemistry*, **2020**, 59, 12802-12816	5.1	4
14	A Bis-Acridinium Macrocycle as Multi-Responsive Receptor and Selective Phase-Transfer Agent of Perylene. *Angewandte Chemie*, **2020**, 132, 23406-23412	3.6	4

13	Identification of Zr(iv)-based architectures generated from ligands incorporating the 2,2′-biphenolato unit. *Dalton Transactions*, **2016**, 45, 7998-8007	4.3	4
12	Unexpected aqueous UCST behavior of a cationic comb polymer with pentaarginine side chains. *European Polymer Journal*, **2020**, 125, 109528	5.2	3
11	Interfacial Activity of the Diprotonated 222 Cryptand at the Water/"Oil" Interface Revealed by Molecular Dynamics Simulations. *Supramolecular Chemistry*, **2003**, 15, 133-142	1.8	3
10	Evaluation of the stereoselectivity for titanium(IV)-based coordination entities induced by the enantiopure diphenylethene-1,2-diamine ligand. *Inorganica Chimica Acta*, **2019**, 498, 119119	2.7	2
9	Interactions between Keggin Anions in Water: The Higher Their Charge, the Higher Their Condensation? A Simulation Study. *European Journal of Inorganic Chemistry*, **2013**, 2013, 1556-1556	2.3	2
8	THE CONTINUING SEARCH FOR LARGE ELITE PRIMES. *International Journal of Number Theory*, **2009**, 05, 209-218	0.5	2
7	Reversible Soft Mechanochemical Control of Biaryl Conformations through Crosslinking in a 3D Macromolecular Network. *Angewandte Chemie*, **2020**, 132, 23483-23490	3.6	2
6	Reversible Soft Mechanochemical Control of Biaryl Conformations through Crosslinking in a 3D Macromolecular Network. *Angewandte Chemie - International Edition*, **2020**, 59, 23283-23290	16.4	2
5	Cold-spray ionization mass spectrometry of the choline chloride-urea deep eutectic solvent (reline). *Journal of Mass Spectrometry*, **2021**, 56, e4725	2.2	2
4	Chemistry on the Complex: Derivatization of TiO N -Based Complexes and Application to Multi-Step Synthesis. *Chemistry - A European Journal*, **2021**, 27, 17910	4.8	1
3	Hydrogen Bonding and Vaporization Thermodynamics in Hexafluoroisopropanol-Acetone and -Methanol Mixtures. A Joined Cluster Analysis and Molecular Dynamic Study. *ChemPhysChem*, **2021**,	3.2	1
2	Symmetry Decrease between Self-Assembled Circular TiO4N2-Based Helicates. *European Journal of Inorganic Chemistry*, **2020**, 2020, 3527-3531	2.3	1
1	The Motion of an Azobenzene Light-Controlled Switch: A Joint Theoretical and Experimental Approach. *ChemSystemsChem*, **2019**, 1, e1900003	3.1	0