Mathieu Salanne

List of Publications by Year in Descending Order

170 papers	8,302 citations	44 h-index	86 g-index
196 ext. papers	9,755 ext. citations	6.7 avg, IF	6.47 L-index

#	Paper	IF	Citations
170	Multi-scale simulation of the adsorption of lithium ion on graphite surface: From quantum Monte Carlo to molecular density functional theory.. *Journal of Chemical Physics*, **2022**, 156, 094709	3.9	0
169	Microscopic Simulations of Electrochemical Double-Layer Capacitors.. *Chemical Reviews*, **2022**,	68.1	5
168	Effects of fluoride salt addition to the physico-chemical properties of the MgCl2NaClKCl heat transfer fluid: A molecular dynamics study. *Solar Energy Materials and Solar Cells*, **2022**, 239, 111649	6.4	0
167	Structure and dynamics of aqueous NaCl solutions at high temperatures and pressures. *Journal of Chemical Physics*, **2021**, 155, 194506	3.9	1
166	Metal-Ion Oligomerization Inside Electrified Carbon Micropores and its Effect on Capacitive Charge Storage. *Advanced Materials*, **2021**, e2107439	24	5
165	Molecular Simulation of Electrode-Solution Interfaces. *Annual Review of Physical Chemistry*, **2021**, 72, 189-212	15.7	24
164	Size dependence of hydrophobic hydration at electrified gold/water interfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	13
163	Computational Amperometry of Nanoscale Capacitors in Molecular Simulations. *Journal of Physical Chemistry Letters*, **2021**, 12, 4357-4361	6.4	5
162	Anion Specific Effects Drive the Formation of Li-Salt Based Aqueous Biphasic Systems. *Journal of Physical Chemistry B*, **2021**, 125, 5365-5372	3.4	2
161	Computational Screening of the Physical Properties of Water-in-Salt Electrolytes**. *Batteries and Supercaps*, **2021**, 4, 646-652	5.6	7
160	Confining Water in Ionic and Organic Solvents to Tune Its Adsorption and Reactivity at Electrified Interfaces. *Accounts of Chemical Research*, **2021**, 54, 1034-1042	24.3	7
159	Effect of the metallicity on the capacitance of gold-aqueous sodium chloride interfaces. *Journal of Chemical Physics*, **2021**, 155, 044703	3.9	5
158	Solvation of anthraquinone and TEMPO redox-active species in acetonitrile using a polarizable force field. *Journal of Chemical Physics*, **2021**, 155, 074504	3.9	4
157	Bottom-Up Design of Configurable Oligomer-Derived Conducting Metallopolymers for High-Power Electrochemical Energy Storage. *ACS Nano*, **2021**, 15, 15422-15428	16.7	1
156	A semiclassical Thomas-Fermi model to tune the metallicity of electrodes in molecular simulations. *Journal of Chemical Physics*, **2020**, 153, 174704	3.9	19
155	Mass-zero constrained molecular dynamics for electrode charges in simulations of electrochemical systems. *Journal of Chemical Physics*, **2020**, 152, 194701	3.9	6
154	Competitive Salt Precipitation/Dissolution During Free-Water Reduction in Water-in-Salt Electrolyte. *Angewandte Chemie - International Edition*, **2020**, 59, 15913-15917	16.4	28

153	Competitive Salt Precipitation/Dissolution During Free-Water Reduction in Water-in-Salt Electrolyte. *Angewandte Chemie*, **2020**, 132, 16047-16051	3.6	11
152	Solvent-Solvent Correlations across Graphene: The Effect of Image Charges. *ACS Nano*, **2020**, 14, 7987-7998	13.7	11
151	Investigation of ionic local structure in molten salt fast reactor LiF-ThF4-UF4 fuel by EXAFS experiments and molecular dynamics simulations. *Journal of Molecular Liquids*, **2020**, 307, 112927	6	12
150	A first-principles computational comparison of defect-free and disordered, fluorinated anatase TiO (001) interfaces with water.. *RSC Advances*, **2020**, 10, 8982-8988	3.7	2
149	First-Principles Determination of Transference Numbers in Cryolitic Melts. *Industrial & Engineering Chemistry Research*, **2020**, 59, 13305-13314	3.9	3
148	A first-principles investigation of the structural and electrochemical properties of biredox ionic species in acetonitrile. *Physical Chemistry Chemical Physics*, **2020**, 22, 10561-10568	3.6	5
147	MetalWalls: A classical molecular dynamics software dedicated to the simulation of electrochemical systems. *Journal of Open Source Software*, **2020**, 5, 2373	5.2	26
146	Charge fluctuations from molecular simulations in the constant-potential ensemble. *Physical Chemistry Chemical Physics*, **2020**, 22, 10480-10489	3.6	30
145	Comparing the performance of sulfonium and phosphonium ionic liquids as electrolytes for supercapacitors by molecular dynamics simulations. *Electrochimica Acta*, **2020**, 364, 137181	6.7	5
144	Structural and dynamic properties of soda-lime-silica in the liquid phase. *Journal of Chemical Physics* , **2020**, 153, 214505	3.9	4
143	Tuning water reduction through controlled nanoconfinement within an organic liquid matrix. *Nature Catalysis*, **2020**, 3, 656-663	36.5	38
142	Study of a water-graphene capacitor with molecular density functional theory. *Journal of Chemical Physics*, **2019**, 151, 124111	3.9	19
141	A molecular density functional theory approach to electron transfer reactions. *Chemical Science*, **2019**, 10, 2130-2143	9.4	20
140	Structural, Dynamic, and Thermodynamic Study of KF–AlF3 Melts by Combining High-Temperature NMR and Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2019**, 123, 2147-2156	3.8	6
139	Effect of the carbon microporous structure on the capacitance of aqueous supercapacitors. *Energy Storage Materials*, **2019**, 21, 190-195	19.4	26
138	Pressure induced structural transformations in amorphous MgSiO3 and CaSiO3. *Journal of Non-Crystalline Solids: X*, **2019**, 3, 100024	2.5	11
137	Study of the Partial Charge Transport Properties in the Molten Alumina via Molecular Dynamics. *ACS Omega*, **2019**, 4, 8022-8030	3.9	6
136	Molecular Dynamics Simulations of Ether-Modified Phosphonium Ionic Liquid Confined in between Planar and Porous Graphene Electrode Models. *Journal of Physical Chemistry C*, **2019**, 123, 10816-10825	3.8	16

135	Chasing Aqueous Biphasic Systems from Simple Salts by Exploring the LiTFSI/LiCl/HO Phase Diagram. *ACS Central Science*, **2019**, 5, 640-643	16.8	18
134	Simulating Electrochemical Systems by Combining the Finite Field Method with a Constant Potential Electrode. *Physical Review Letters*, **2019**, 123, 195501	7.4	30
133	Transport Properties of Li-TFSI Water-in-Salt Electrolytes. *Journal of Physical Chemistry B*, **2019**, 123, 10514-10521	3.4	39
132	A New Electrolyte Formulation for Securing High Temperature Cycling and Storage Performances of Na-Ion Batteries. *Advanced Energy Materials*, **2019**, 9, 1901431	21.8	26
131	In situ high-temperature EXAFS measurements on radioactive and air-sensitive molten salt materials. *Journal of Synchrotron Radiation*, **2019**, 26, 124-136	2.4	13
130	Many-body effects at the origin of structural transitions in BO. *Journal of Chemical Physics*, **2019**, 151, 224508	3.9	0
129	Impact of Anion Vacancies on the Local and Electronic Structures of Iron-Based Oxyfluoride Electrodes. *Journal of Physical Chemistry Letters*, **2019**, 10, 107-112	6.4	10
128	Performance of microporous carbon electrodes for supercapacitors: Comparing graphene with disordered materials. *Energy Storage Materials*, **2019**, 17, 88-92	19.4	30
127	Blue Energy and Desalination with Nanoporous Carbon Electrodes: Capacitance from Molecular Simulations to Continuous Models. *Physical Review X*, **2018**, 8,	9.1	15
126	On the determination of ion transport numbers in molten salts using molecular dynamics. *Electrochimica Acta*, **2018**, 274, 266-273	6.7	15
125	Materials for supercapacitors: When Li-ion battery power is not enough. *Materials Today*, **2018**, 21, 419-436	23.8	234
124	Ion-ion correlations across and between electrified graphene layers. *Journal of Chemical Physics*, **2018**, 148, 193812	3.9	22
123	Computer simulation studies of nanoporous carbon-based electrochemical capacitors. *Current Opinion in Electrochemistry*, **2018**, 9, 81-86	7.2	13
122	Structural study of Na2O-B2O3-SiO2-La2O3 glasses from molecular simulations using a polarizable force field. *Journal of Non-Crystalline Solids*, **2018**, 499, 371-379	3.9	13
121	Classical Polarizable Force Field to Study Hydrated Hectorite: Optimization on DFT Calculations and Validation against XRD Data. *Minerals (Basel, Switzerland)*, **2018**, 8, 205	2.4	8
120	Insights into Li+, Na+, and K+ Intercalation in Lepidocrocite-Type Layered TiO2 Structures. *ACS Applied Energy Materials*, **2018**, 1, 2078-2086	6.1	21
119	The Fate of Water at the Electrochemical Interfaces: Electrochemical Behavior of Free Water Versus Coordinating Water. *Journal of Physical Chemistry Letters*, **2018**, 9, 6683-6688	6.4	55
118	Classical Polarizable Force Field To Study Hydrated Charged Clays and Zeolites. *Journal of Physical Chemistry C*, **2018**, 122, 24690-24704	3.8	9

117	Capacitive Performance of Water-in-Salt Electrolytes in Supercapacitors: A Simulation Study. *Journal of Physical Chemistry C*, **2018**, 122, 23917-23924	3.8	31
116	Anionic Structure in Molten Cryolite–Alumina Systems. *Journal of Physical Chemistry C*, **2018**, 122, 21807-21816	3.8	9
115	Probing ice VII crystallization from amorphous NaCl-DO solutions at gigapascal pressures. *Physical Chemistry Chemical Physics*, **2017**, 19, 1875-1883	3.6	13
114	Confinement Effects on an Electron Transfer Reaction in Nanoporous Carbon Electrodes. *Journal of Physical Chemistry Letters*, **2017**, 8, 1925-1931	6.4	26
113	Study of NaF–AlF3 Melts by Coupling Molecular Dynamics, Density Functional Theory, and NMR Measurements. *Journal of Physical Chemistry C*, **2017**, 121, 10289-10297	3.8	21
112	Classical Polarizable Force Field To Study Dry Charged Clays and Zeolites. *Journal of Physical Chemistry C*, **2017**, 121, 9833-9846	3.8	11
111	Ca -Cl Association in Water Revisited: the Role of Cation Hydration. *ChemPhysChem*, **2017**, 18, 2807-2811	3.2	9
110	Ionic Liquids for Supercapacitor Applications. *Topics in Current Chemistry*, **2017**, 375, 63	7.2	82
109	Partial breaking of the Coulombic ordering of ionic liquids confined in carbon nanopores. *Nature Materials*, **2017**, 16, 1225-1232	27	166
108	Reversible magnesium and aluminium ions insertion in cation-deficient anatase TiO. *Nature Materials*, **2017**, 16, 1142-1148	27	270
107	Layered Lepidocrocite Type Structure Isolated by Revisiting the Sol–Gel Chemistry of Anatase TiO2: A New Anode Material for Batteries. *Chemistry of Materials*, **2017**, 29, 8313-8324	9.6	25
106	Structural study of NaO-BO-SiO glasses from molecular simulations using a polarizable force field. *Journal of Chemical Physics*, **2017**, 147, 161711	3.9	22
105	Navigating at Will on the Water Phase Diagram. *Physical Review Letters*, **2017**, 119, 245701	7.4	30
104	Ionic Liquids for Supercapacitor Applications. *Topics in Current Chemistry Collections*, **2017**, 29-53	1.8	9
103	Dynamic Response in Nanoelectrowetting on a Dielectric. *ACS Nano*, **2016**, 10, 8536-44	16.7	25
102	Sparse Cyclic Excitations Explain the Low Ionic Conductivity of Stoichiometric Li_{7}La_{3}Zr_{2}O_{12}. *Physical Review Letters*, **2016**, 116, 135901	7.4	41
101	Collective water dynamics in the first solvation shell drive the NMR relaxation of aqueous quadrupolar cations. *Journal of Chemical Physics*, **2016**, 145, 124508	3.9	7
100	Molecular Dynamics Simulations of the Influence of Drop Size and Surface Potential on the Contact Angle of Ionic-Liquid Droplets. *Journal of Physical Chemistry C*, **2016**, 120, 15244-15250	3.8	44

99	Coordination numbers and physical properties in molten salts and their mixtures. *Faraday Discussions*, **2016**, 190, 471-86	3.6	24
98	Understanding the different (dis)charging steps of supercapacitors: influence of potential and solvation. *Electrochimica Acta*, **2016**, 206, 504-512	6.7	15
97	Classical Polarizable Force Field for Clays: Pyrophyllite and Talc. *Journal of Physical Chemistry C*, **2016**, 120, 3749-3758	3.8	25
96	Multi-scale modelling of supercapacitors: From molecular simulations to a transmission line model. *Journal of Power Sources*, **2016**, 326, 680-685	8.9	36
95	Capacitance of Nanoporous Carbon-Based Supercapacitors Is a Trade-Off between the Concentration and the Separability of the Ions. *Journal of Physical Chemistry Letters*, **2016**, 7, 4015-4021	6.4	62
94	A DFT-Based Aspherical Ion Model for Sodium Aluminosilicate Glasses and Melts. *Journal of Physical Chemistry C*, **2016**, 120, 24370-24381	3.8	14
93	Formulation of Temperature-Dependent Thermal Conductivity of NaF, □Na3AlF6, Na5Al3F14, and Molten Na3AlF6 Supported by Equilibrium Molecular Dynamics and Density Functional Theory. *Journal of Physical Chemistry C*, **2016**, 120, 22873-22886	3.8	20
92	Thorium Molten Salts: Theory and Practice **2016**, 111-116		
91	Efficient storage mechanisms for building better supercapacitors. *Nature Energy*, **2016**, 1,	62.3	1256
90	Molecular Dynamics Simulations of Electrochemical Energy Storage Devices. *Green Energy and Technology*, **2016**, 61-89	0.6	3
89	Simulations of room temperature ionic liquids: from polarizable to coarse-grained force fields. *Physical Chemistry Chemical Physics*, **2015**, 17, 14270-9	3.6	120
88	High Substitution Rate in TiO2 Anatase Nanoparticles with Cationic Vacancies for Fast Lithium Storage. *Chemistry of Materials*, **2015**, 27, 5014-5019	9.6	66
87	Tuning the Electronic Structure of Anatase Through Fluorination. *Scientific Reports*, **2015**, 5, 11553	4.9	13
86	Structural characterization of eutectic aqueous NaCl solutions under variable temperature and pressure conditions. *Physical Chemistry Chemical Physics*, **2015**, 17, 14054-63	3.6	16
85	Anionic ordering and thermal properties of FeF3□3H2O. *Inorganic Chemistry*, **2015**, 54, 9619-25	5.1	17
84	DFT-based polarizable force field for TiO2and SiO2. *Modelling and Simulation in Materials Science and Engineering*, **2015**, 23, 074005	2	8
83	Toward an Accurate Modeling of Ionic Liquid□TiO2 Interfaces. *Journal of Physical Chemistry C*, **2015**, 119, 25260-25267	3.8	19
82	Transport coefficients and the Stokes□Einstein relation in molten alkali halides with polarisable ion model. *Molecular Physics*, **2015**, 113, 2442-2450	1.7	22

81	Confinement, Desolvation, And Electrosorption Effects on the Diffusion of Ions in Nanoporous Carbon Electrodes. *Journal of the American Chemical Society*, **2015**, 137, 12627-32	16.4	116
80	Structural Transitions at Ionic Liquid Interfaces. *Journal of Physical Chemistry Letters*, **2015**, 6, 4978-85	6.4	73
79	Thermal transport properties of halide solid solutions: Experiments vs equilibrium molecular dynamics. *Journal of Chemical Physics*, **2015**, 142, 124109	3.9	14
78	On the microscopic fluctuations driving the NMR relaxation of quadrupolar ions in water. *Journal of Chemical Physics*, **2015**, 143, 194504	3.9	13
77	Liquid B2O3 up to 1700 K: x-ray diffraction and boroxol ring dissolution. *Journal of Physics Condensed Matter*, **2015**, 27, 455104	1.8	22
76	Molecular aspects of the Eu3+/Eu2+ redox reaction at the interface between a molten salt and a metallic electrode. *Molecular Physics*, **2015**, 113, 2451-2462	1.7	9
75	Single Electrode Capacitances of Porous Carbons in Neat Ionic Liquid Electrolyte at 100°C: A Combined Experimental and Modeling Approach. *Journal of the Electrochemical Society*, **2015**, 162, A5091-A5095	3.9	23
74	In Situ Experimental Approach of Speciation in Molten Fluorides: A Combination of NMR, EXAFS, and Molecular Dynamics **2014**, 219-228		2
73	On the dynamics of charging in nanoporous carbon-based supercapacitors. *ACS Nano*, **2014**, 8, 1576-83	16.7	151
72	Structure of tetraalkylammonium ionic liquids in the interlayer of modified montmorillonite. *Journal of Physics Condensed Matter*, **2014**, 26, 284107	1.8	5
71	Multiscale modelling of transport in clays from the molecular to the sample scale. *Comptes Rendus - Geoscience*, **2014**, 346, 298-306	1.4	9
70	The Electric Double Layer Has a Life of Its Own. *Journal of Physical Chemistry C*, **2014**, 118, 18291-18298	3.8	161
69	The effect of dispersion interactions on the properties of LiF in condensed phases. *Journal of Physics Condensed Matter*, **2014**, 26, 244103	1.8	6
68	Prediction of the thermophysical properties of molten salt fast reactor fuel from first-principles. *Molecular Physics*, **2014**, 112, 1305-1312	1.7	34
67	Thermal conductivity of molten alkali metal fluorides (LiF, NaF, KF) and their mixtures. *Journal of Physical Chemistry B*, **2014**, 118, 3385-91	3.4	34
66	Ceria co-doping: synergistic or average effect?. *Physical Chemistry Chemical Physics*, **2014**, 16, 8320-31	3.6	60
65	Structure and Dynamics of Alkali and Alkaline Earth Molten Fluorides by High-Temperature NMR and Molecular Dynamics **2014**, 235-241		
64	Molten Salts: from First Principles to Material Properties **2014**, 159-162		

63	Pierre Turq, an inspirational scientist in charge and at interfaces. *Molecular Physics*, **2014**, 112, 1213-1221	1.7	
62	Coarse graining the dynamics of nano-confined solutes: the case of ions in clays. *Molecular Simulation*, **2014**, 40, 237-244	2	13
61	Accurate quadrupolar NMR relaxation rates of aqueous cations from classical molecular dynamics. *Journal of Physical Chemistry B*, **2014**, 118, 13252-7	3.4	12
60	Thermal conductivity of simple liquids: origin of temperature and packing fraction dependences. *Journal of Chemical Physics*, **2014**, 140, 114502	3.9	10
59	Density-driven structural transformations in B2O3 glass. *Physical Review B*, **2014**, 90,	3.3	42
58	Computer simulations of ionic liquids at electrochemical interfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 15781-92	3.6	133
57	Molecular dynamics simulation of the thermodynamic and transport properties of the molten salt fast reactor fuel LiF□ThF4. *Journal of Nuclear Materials*, **2013**, 434, 322-327	3.3	42
56	Modeling of Molten Salts **2013**, 1-16		7
55	Charge fluctuations in nanoscale capacitors. *Physical Review Letters*, **2013**, 111, 106102	7.4	97
54	Highly confined ions store charge more efficiently in supercapacitors. *Nature Communications*, **2013**, 4, 2701	17.4	328
53	Is a Stern and diffuse layer model appropriate to ionic liquids at surfaces?. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, E4121	11.5	84
52	Effects of Li-ion vacancies on the ionic conduction mechanism of LiMgSO4F. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 074003	2	2
51	Molecular dynamics simulations of Y in silicate melts and implications for trace element partitioning. *Chemical Geology*, **2013**, 346, 14-21	4.2	18
50	Vibrational Sum Frequency Generation Spectroscopy of the Water Liquid-Vapor Interface from Density Functional Theory-Based Molecular Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2013**, 4, 83-7	6.4	128
49	Simulating Supercapacitors: Can We Model Electrodes As Constant Charge Surfaces?. *Journal of Physical Chemistry Letters*, **2013**, 4, 264-8	6.4	170
48	A comprehensive study of the heat capacity of CsF from T=5K to T=1400K. *Journal of Chemical Thermodynamics*, **2013**, 57, 92-100	2.9	12
47	Candidate molten salt investigation for an accelerator driven subcritical core. *Journal of Nuclear Materials*, **2013**, 440, 298-303	3.3	18
46	Influence of solvation on the structural and capacitive properties of electrical double layer capacitors. *Electrochimica Acta*, **2013**, 101, 262-271	6.7	83

45	Structure and dynamics in yttrium-based molten rare earth alkali fluorides. *Journal of Chemical Physics*, **2013**, 138, 184503	3.9	30
44	Structural effects on the electrical conductivity of molten fluorides: Comparison between LiF YF3 and LiF NaF ZrF4. *Journal of Fluorine Chemistry*, **2012**, 134, 44-48	2.1	10
43	Cooperative Mechanism for the Diffusion of Li+ Ions in LiMgSO4F. *Journal of Physical Chemistry C*, **2012**, 116, 18618-18625	3.8	40
42	New Coarse-Grained Models of Imidazolium Ionic Liquids for Bulk and Interfacial Molecular Simulations. *Journal of Physical Chemistry C*, **2012**, 116, 7687-7693	3.8	104
41	Absolute acidity of clay edge sites from ab-initio simulations. *Geochimica Et Cosmochimica Acta*, **2012**, 94, 1-11	5.5	74
40	Thermal conductivity of MgO, MgSiO3 perovskite and post-perovskite in the Earth's deep mantle. *Earth and Planetary Science Letters*, **2012**, 355-356, 102-108	5.3	48
39	Diffusion coefficient and shear viscosity of rigid water models. *Journal of Physics Condensed Matter*, **2012**, 24, 284117	1.8	73
38	On the molecular origin of supercapacitance in nanoporous carbon electrodes. *Nature Materials*, **2012**, 11, 306-10	27	728
37	Including many-body effects in models for ionic liquids. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	97
36	From molten salts to room temperature ionic liquids: simulation studies on chloroaluminate systems. *Faraday Discussions*, **2012**, 154, 171-88; discussion 189-220, 465-71	3.6	47
35	Car-Parrinello molecular dynamics study of the uranyl behaviour at the gibbsite/water interface. *Journal of Chemical Physics*, **2012**, 137, 154705	3.9	12
34	A transferable ab initio based force field for aqueous ions. *Journal of Chemical Physics*, **2012**, 136, 114507	3.9	54
33	Ions in solutions: Determining their polarizabilities from first-principles. *Journal of Chemical Physics*, **2011**, 134, 014511	3.9	57
32	Ion specific effects on the structure of molten AF-ZrF4 systems (A+ = Li+, Na+, and K+). *Journal of Physical Chemistry B*, **2011**, 115, 9160-7	3.4	58
31	Studies of the local structures of molten metal halides. *Annual Reports on the Progress of Chemistry Section C*, **2011**, 107, 88		67
30	Imidazolium Ionic Liquid Interfaces with Vapor and Graphite: Interfacial Tension and Capacitance from Coarse-Grained Molecular Simulations. *Journal of Physical Chemistry C*, **2011**, 115, 16613-16618	3.8	123
29	Primitive models of ions in solution from molecular descriptions: a perturbation approach. *Journal of Chemical Physics*, **2011**, 135, 234509	3.9	26
28	Thermal conductivity of ionic systems from equilibrium molecular dynamics. *Journal of Physics Condensed Matter*, **2011**, 23, 102101	1.8	26

27	Polarization effects in ionic solids and melts. *Molecular Physics*, **2011**, 109, 2299-2315	1.7	107
26	Optical basicity scales in protic solvents: water, hydrogen fluoride, ammonia and their mixtures. *Physical Chemistry Chemical Physics*, **2011**, 13, 6305-8	3.6	8
25	Transport Properties in Cryolitic Melts: NMR Measurements and Molecular Dynamics Calculations of Self-Diffusion Coefficients. *ECS Transactions*, **2010**, 33, 679-684	1	6
24	Investigation of Fluoroacidity in Molten Fluorides by the Combination of High Temperature NMR and Molecular Dynamics. *ECS Transactions*, **2010**, 33, 159-165	1	3
23	From localized orbitals to material properties: building classical force fields for nonmetallic condensed matter systems. *Physical Review Letters*, **2010**, 104, 138301	7.4	32
22	High-pressure behaviour of GeO2: a simulation study. *Journal of Physics Condensed Matter*, **2010**, 22, 152102	1.8	46
21	In Situ Experimental Approach of the Speciation in Molten Lanthanide and Actinide Fluorides Combining NMR, EXAFS and Molecular Dynamics. *ECS Transactions*, **2010**, 33, 361-369	1	2
20	Potential-induced ordering transition of the adsorbed layer at the ionic liquid/electrified metal interface. *Journal of Physical Chemistry B*, **2010**, 114, 8453-9	3.4	83
19	In situ experimental evidence for a nonmonotonous structural evolution with composition in the molten LiF-ZrF4 system. *Journal of Physical Chemistry B*, **2010**, 114, 6472-9	3.4	55
18	Internal mobilities and diffusion in an ionic liquid mixture. *Physical Chemistry Chemical Physics*, **2010**, 12, 14109-14	3.6	21
17	Models of electrolyte solutions from molecular descriptions: the example of NaCl solutions. *Physical Review E*, **2009**, 80, 065103	2.4	23
16	Calculations of the thermal conductivities of ionic materials by simulation with polarizable interaction potentials. *Journal of Chemical Physics*, **2009**, 130, 104507	3.9	64
15	Density functional theory, molecular dynamics, and differential scanning calorimetry study of the RbF-CsF phase diagram. *Journal of Chemical Physics*, **2009**, 130, 134716	3.9	13
14	Transport in molten LiF□NaF□rF4 mixtures: A combined computational and experimental approach. *Journal of Fluorine Chemistry*, **2009**, 130, 61-66	2.1	28
13	Heat-transport properties of molten fluorides: Determination from first-principles. *Journal of Fluorine Chemistry*, **2009**, 130, 38-44	2.1	78
12	The construction of a reliable potential for GeO2 from first principles. *Molecular Physics*, **2009**, 107, 443-452	1.7	40
11	Ion adsorption at a metallic electrode: an ab initio based simulation study. *Journal of Physics Condensed Matter*, **2009**, 21, 424109	1.8	38
10	Diffusion coefficients and local structure in basic molten fluorides: in situ NMR measurements and molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2009**, 11, 11501-6	3.6	55

9	Intermediate range chemical ordering of cations in simple molten alkali halides. *Journal of Physics Condensed Matter*, **2008**, 20, 332101	1.8	22
8	Calculation of activities of ions in molten salts with potential application to the pyroprocessing of nuclear waste. *Journal of Physical Chemistry B*, **2008**, 112, 1177-83	3.4	82
7	Polarizabilities of individual molecules and ions in liquids from first principles. *Journal of Physics Condensed Matter*, **2008**, 20, 494207	1.8	36
6	Simulation of the liquid□apor interface of molten LiBeF3. *Comptes Rendus Chimie*, **2007**, 10, 1131-1136	2.7	17
5	Role of elemental fluorine in nuclear field. *Journal of Fluorine Chemistry*, **2007**, 128, 285-295	2.1	13
4	Conductivity-viscosity-structure: unpicking the relationship in an ionic liquid. *Journal of Physical Chemistry B*, **2007**, 111, 4678-84	3.4	88
3	A first-principles description of liquid BeF2 and its mixtures with LiF: 2. Network formation in LiF-BeF2. *Journal of Physical Chemistry B*, **2006**, 110, 11461-7	3.4	86
2	A first-principles description of liquid BeF2 and its mixtures with LiF: 1. Potential development and pure BeF2. *Journal of Physical Chemistry B*, **2006**, 110, 11454-60	3.4	90
1	Molecular dynamics simulation of hydrogen fluoride mixtures with 1-ethyl-3-methylimidazolium fluoride: a simple model for the study of structural features. *Journal of Physical Chemistry B*, **2006**, 110, 3504-10	3.4	17