Milan PÅedota

List of Publications by Year
in descending order

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50 papers	2,151 citations	257357 24 h-index	223716 46 g-index
50 all docs	50 docs citations	50 times ranked	2010 citing authors

#	Article	IF	Citations
1	The â€œgood,â€• the â€œbad,â€• and the â€œhiddenâ€• in neutron scattering and molecular dynamics of ionic aqueous solutions. Journal of Chemical Physics, 2022, 156, .	1.2	6
2	Local molecular environment drives speciation and reactivity of ion complexes in concentrated salt solution. Journal of Molecular Liquids, 2021, 340, 116898.	2.3	8
3	Clinoptilolite/electrolyte interface probed by a classical molecular dynamics simulations and batch adsorption experiments. Microporous and Mesoporous Materials, 2021, 328, 111406.	2.2	1
4	Second Harmonic Scattering Reveals Ion-Specific Effects at the SiO₂ and TiO₂ Nanoparticle/Aqueous Interface. Journal of Physical Chemistry C, 2021, 125, 25261-25274.	1.5	11
5	Zeta Potential Determination from Molecular Simulations. Journal of Physical Chemistry C, 2020, 124, 3159-3170.	1.5	39
6	Phase-Sensitive Vibrational SFG Spectra from Simple Classical Force Field Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2020, 124, 15253-15263.	1.5	9
7	Electronic continuum correction without scaled charges. Journal of Molecular Liquids, 2020, 314, 113571.	2.3	10
8	Surface Potential and Interfacial Water Order at the Amorphous TiO₂Nanoparticle/Aqueous Interface. Journal of Physical Chemistry C, 2020, 124, 10961-10974.	1.5	25
9	Surface Characterization of Colloidal Silica Nanoparticles by Second Harmonic Scattering: Quantifying the Surface Potential and Interfacial Water Order. Journal of Physical Chemistry C, 2019, 123, 20393-20404.	1.5	36
10	Oxalic Acid Adsorption on Rutile: Molecular Dynamics and ab Initio Calculations. Langmuir, 2019, 35, 7617-7630.	1.6	13
11	Oxalic Acid Adsorption on Rutile: Experiments and Surface Complexation Modeling to 150 Â°C. Langmuir, 2019, 35, 7631-7640.	1.6	6
12	Quartz/Aqueous Electrolyte Solution Interface: Molecular Dynamic Simulation and Interfacial Potential Measurements. Journal of Physical Chemistry C, 2018, 122, 24025-24036.	1.5	30
13	Modeling of solidâ€“liquid interfaces using scaled charges: rutile (110) surfaces. Physical Chemistry Chemical Physics, 2018, 20, 23954-23966.	1.3	29
14	Force field parametrization of hydrogenoxalate and oxalate anions with scaled charges. Journal of Molecular Modeling, 2017, 23, 327.	0.8	19
15	Molecular Origins of the Zeta Potential. Langmuir, 2016, 32, 10189-10198.	1.6	90
16	PtÂ·Â·Â·H Nonclassical Interaction in Water-Dissolved Pt(II) Complexes: Coaction of Electronic Effects with Solvent-Assisted Stabilization. Inorganic Chemistry, 2016, 55, 3252-3264.	1.9	13
17	Constrained Surface Complexation Modeling: Rutile in RbCl, NaCl, and NaCF₃SO₃ Media to 250 Â°C. Journal of Physical Chemistry C, 2015, 119, 15204-15215.	1.5	12
18	Computer Simulations of Quartz (101)â€“Water Interface over a Range of pH Values. Journal of Physical Chemistry C, 2015, 119, 9274-9286.	1.5	99

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19	Dielectric Properties of Water at Rutile and Graphite Surfaces: Effect of Molecular Structure. Journal of Physical Chemistry C, 2014, 118, 4818-4834.	1.5	51
20	Electric Double Layer at the Rutile (110) Surface. 4. Effect of Temperature and pH on the Adsorption and Dynamics of Ions. Journal of Physical Chemistry C, 2013, 117, 22852-22866.	1.5	34
21	Molecular-level simulations of chemical reaction equilibrium and diffusion in slit and cylindrical nanopores: model dimerisation reactions. Molecular Simulation, 2013, 39, 1103-1120.	0.9	13
22	Comment on â€œStructure and dynamics of liquid water on rutile TiO2(110)â€• Physical Review B, 2012, 85, .	1.1	46
23	Influence of a charged graphene surface on the orientation and conformation of covalently attached oligonucleotides: a molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 4217.	1.3	25
24	Determination of the distance-dependent viscosity of mixtures in parallel slabs using non-equilibrium molecular dynamics. Physical Chemistry Chemical Physics, 2012, 14, 3640.	1.3	11
25	Influence of the Environment on the Specificity of the Mg(II) Binding to Uracil. Journal of Physical Chemistry A, 2012, 116, 1786-1793.	1.1	4
26	Comparison of Cation Adsorption by Isostructural Rutile and Cassiterite. Langmuir, 2011, 27, 4585-4593.	1.6	29
27	Coarse-grained potential for interaction with a spherical colloidal particle and planar wall. Collection of Czechoslovak Chemical Communications, 2010, 75, 527-545.	1.0	2
28	Ion Adsorption on Metal Oxide Surfaces to Hydrothermal Conditions.. ECS Transactions, 2008, 11, 167-180.	0.3	7
29	The Protonation Behavior of Metal Oxide Surfaces to Hydrothermal Conditions. ECS Transactions, 2008, 11, 151-166.	0.3	3
30	Surface Protonation at the Rutile (110) Interface: Explicit Incorporation of Solvation Structure within the Refined MUSIC Model Framework. Langmuir, 2008, 24, 12331-12339.	1.6	88
31	Comment on Parts 1 and 2 of the Series â€œElectric Double Layer at the Rutile (110) Surfaceâ€• Journal of Physical Chemistry B, 2007, 111, 1245-1247.	1.2	29
32	Electric Double Layer at Metal Oxide Surfaces:Â Static Properties of the Cassiteriteâˆ’Water Interface. Langmuir, 2007, 23, 4925-4937.	1.6	63
33	Electric Double Layer at the Rutile (110) Surface. 3. Inhomogeneous Viscosity and Diffusivity Measurement by Computer Simulations. Journal of Physical Chemistry C, 2007, 111, 3071-3079.	1.5	78
34	Hydration of apolar solutes of varying size: a systematic study. Molecular Physics, 2006, 104, 2465-2476.	0.8	41
35	From dimer to condensed phases at extreme conditions: Accurate predictions of the properties of water by a Gaussian charge polarizable model. Journal of Chemical Physics, 2005, 122, 244511.	1.2	202
36	Electric Double Layer at the Rutile (110) Surface. 2. Adsorption of Ions from Molecular Dynamics and X-ray Experiments. Journal of Physical Chemistry B, 2004, 108, 12061-12072.	1.2	127

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37	Electric Double Layer at the Rutile (110) Surface. 1. Structure of Surfaces and Interfacial Water from Molecular Dynamics by Use of ab Initio Potentials. Journal of Physical Chemistry B, 2004, 108, 12049-12060.	1.2	272
38	Ion Adsorption at the Rutileâ^'Water Interface:Â Linking Molecular and Macroscopic Properties. Langmuir, 2004, 20, 4954-4969.	1.6	298
39	On independence of the solvation of interaction sites of a water molecule. Journal of Chemical Physics, 2003, 118, 6446-6454.	1.2	13
40	Pair approximation for polarization interaction and adiabatic nuclear and electronic sampling method for fluids with dipole polarizability. Molecular Physics, 2002, 100, 2703-2717.	0.8	14
41	Hydrophobic hydration at the level of primitive models. II: Large solutes and water restructuring. Molecular Physics, 2002, 100, 2189-2200.	0.8	20
42	Vaporâ€“liquid equilibrium simulations of the SCPDP model of water. Chemical Physics Letters, 2002, 357, 189-194.	1.2	56
43	Pair approximation for polarization interaction: efficient method for Monte Carlo simulations of polarizable fluids. Molecular Physics, 2001, 99, 349-354.	0.8	20
44	On the determination of the vaporâ€“liquid envelope for polarizable models by Monte Carlo simulation. Fluid Phase Equilibria, 2001, 183-184, 295-300.	1.4	7
45	Hydrophobic hydration at the level of primitive models. Molecular Physics, 1999, 96, 1237-1248.	0.8	14
46	Hydrophobic hydration at the level of primitive models. Molecular Physics, 1999, 96, 1237-1248.	0.8	8
47	Fluids of pseudo-hard bodies II. Reference models for water, methanol, and ammonia. Molecular Physics, 1998, 94, 937-948.	0.8	20
48	Scaling in a two-component surface-growth model. Physical Review B, 1998, 58, 10003-10011.	1.1	25
49	Interplay between kinetic roughening and phase ordering. Europhysics Letters, 1997, 39, 251-256.	0.7	26
50	Stochastic equations for simple discrete models of epitaxial growth. Physical Review E, 1996, 54, 3933-3942.	0.8	49