Daniel Borgis

List of Publications by Year
in descending order

67 papers	3,768 citations	126708 33 h-index	123241 61 g-index
67 all docs	67 docs citations	67 times ranked	2136 citing authors

#	Article	IF	Citations
1	Quantifying Fluctuations of Average Solvent Environments for Embedding Calculations. Journal of Chemical Theory and Computation, 2022, 18, 1072-1088.	2.3	4
2	Accurate prediction of hydration free energies and solvation structures using molecular density functional theory with a simple bridge functional. Journal of Chemical Physics, 2021, 155, 024117.	1.2	9
3	Tackling Solvent Effects by Coupling Electronic and Molecular Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 7123-7134.	2.3	19
4	Predicting Hydration Free Energies of the FreeSolv Database of Drug-like Molecules with Molecular Density Functional Theory. Journal of Chemical Information and Modeling, 2020, 60, 3558-3565.	2.5	6
5	Simple Parameter-Free Bridge Functionals for Molecular Density Functional Theory. Application to Hydrophobic Solvation. Journal of Physical Chemistry B, 2020, 124, 6885-6893.	1.2	13
6	Hydration free energies and solvation structures with molecular density functional theory in the hypernetted chain approximation. Journal of Chemical Physics, 2020, 152, 064110.	1.2	21
7	Computing three-dimensional densities from force densities improves statistical efficiency. Journal of Chemical Physics, 2019, 151, 064124.	1.2	12
8	Study of a water-graphene capacitor with molecular density functional theory. Journal of Chemical Physics, 2019, 151, 124111.	1.2	31
9	A molecular density functional theory approach to electron transfer reactions. Chemical Science, 2019, 10, 2130-2143.	3.7	24
10	Screened Coulombic Orientational Correlations in Dilute Aqueous Electrolytes. Journal of Physical Chemistry Letters, 2018, 9, 1985-1989.	2.1	22
11	What Does Second-Harmonic Scattering Measure in Diluted Electrolytes?. Journal of Physical Chemistry Letters, 2018, 9, 3698-3702.	2.1	15
12	Electronic Excited State Lifetimes of Anionic Water Clusters: Dependence on Charge Solvation Motif. Journal of Physical Chemistry Letters, 2017, 8, 2304-2309.	2.1	15
13	Efficient molecular density functional theory using generalized spherical harmonics expansions. Journal of Chemical Physics, 2017, 147, 094107.	1.2	29
14	Molecular density functional theory of water including densityâ€“polarization coupling. Journal of Physics Condensed Matter, 2016, 28, 244005.	0.7	15
15	Solvation free-energy pressure corrections in the three dimensional reference interaction site model. Journal of Chemical Physics, 2015, 143, 184116.	1.2	67
16	Molecular density functional theory for water with liquid-gas coexistence and correct pressure. Journal of Chemical Physics, 2015, 142, 154112.	1.2	26
17	Fast Computation of Solvation Free Energies with Molecular Density Functional Theory: Thermodynamic-Ensemble Partial Molar Volume Corrections. Journal of Physical Chemistry Letters, 2014, 5, 1935-1942.	2.1	67
18	Introduction to Classical Density Functional Theory by a Computational Experiment. Journal of Chemical Education, 2014, 91, 2112-2115.	1.1	8

#	Article	IF	Citations
19	Hydration of clays at the molecular scale: the promising perspective of classical density functional theory. Molecular Physics, 2014, 112, 1320-1329.	0.8	11
20	Computing Wigner distributions and time correlation functions using the quantum thermal bath method: application to proton transfer spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 12591.	1.3	32
21	Computation of pair distribution functions and three-dimensional densities with a reduced variance principle. Molecular Physics, 2013, 111, 3486-3492.	0.8	39
22	Molecular density functional theory of water describing hydrophobicity at short and long length scales. Journal of Chemical Physics, 2013, 139, 154101.	1.2	37
23	Molecular Density Functional Theory of Water. Journal of Physical Chemistry Letters, 2013, 4, 619-624.	2.1	76
24	A multiscale coarseâ€grained polarizable solvent model for handling long tail bulk electrostatics. Journal of Computational Chemistry, 2013, 34, 1112-1124.	1.5	17
25	Modeling Proteinâ€“Protein Recognition in Solution Using the Coarse-Grained Force Field SCORPION. Journal of Chemical Theory and Computation, 2013, 9, 803-813.	2.3	47
26	Molecular Density Functional Theory: Application to Solvation and Electron-Transfer Thermodynamics in Polar Solvents. Journal of Physical Chemistry B, 2012, 116, 2504-2512.	1.2	42
27	Extension of Marcus Picture for Electron Transfer Reactions with Large Solvation Changes. Journal of the American Chemical Society, 2012, 134, 2067-2074.	6.6	42
28	Solvation of complex surfaces via molecular density functional theory. Journal of Chemical Physics, 2012, 137, 224107.	1.2	23
29	Hopping along hydrogen bonds. Nature Chemistry, 2012, 4, 432-433.	6.6	46
30	Scalar fundamental measure theory for hard spheres in three dimensions: Application to hydrophobic solvation. Journal of Chemical Physics, 2012, 137, 034115.	1.2	42
31	Molecular density functional theory of solvation: From polar solvents to water. Journal of Chemical Physics, 2011, 134, 194102.	1.2	86
32	Combining a polarizable forceâ€field and a coarseâ€grained polarizable solvent model. II. Accounting for hydrophobic effects. Journal of Computational Chemistry, 2011, 32, 2664-2678.	1.5	28
33	A polarizable coarse-grained water model for coarse-grained proteins simulations. Chemical Physics Letters, 2009, 468, 79-82.	1.2	42
34	Classical density functional theory of solvation in molecular solvents: Angular grid implementation. Chemical Physics Letters, 2009, 474, 366-370.	1.2	49
35	Combining a polarizable forceâ€field and a coarseâ€grained polarizable solvent model: Application to long dynamics simulations of bovine pancreatic trypsin inhibitor. Journal of Computational Chemistry, 2008, 29, 1707-1724.	1.5	42
36	Nuclear quantum effects on the nonadiabatic decay mechanism of an excited hydrated electron. Journal of Chemical Physics, 2007, 127, 174508.	1.2	29

#	Article	IF	Citations
37	A Coarse-Grained Proteinâ"Protein Potential Derived from an All-Atom Force Field. Journal of Physical Chemistry B, 2007, 111, 9390-9399.	1.2	92
38	Coarse-Graining the Accessible Surface and the Electrostatics of Proteins for Proteinâ"Protein Interactions. Journal of Chemical Theory and Computation, 2007, 3, 1867-1876.	2.3	9
39	Particle-Based Implicit Solvent Model for Biosimulations:â€‰ Application to Proteins and Nucleic Acids Hydration. Journal of Chemical Theory and Computation, 2006, 2, 1646-1656.	2.3	20
40	Generating approximate Wigner distributions using Gaussian phase packets propagation in imaginary time. Chemical Physics Letters, 2006, 423, 390-394.	1.2	15
41	Direct correlation functions and the density functional theory of polar solvents. Chemical Physics, 2005, 319, 261-272.	0.9	38
42	A dielectric continuum model of solvation for complex solutes. Computer Physics Communications, 2005, 169, 69-74.	3.0	9
43	Density Functional Theory of Solvation and Its Relation to Implicit Solvent Modelsâ€. Journal of Physical Chemistry B, 2005, 109, 6754-6763.	1.2	74
44	A semi-implicit solvent model for the simulation of peptides and proteins. Journal of Computational Chemistry, 2004, 25, 1015-1029.	1.5	22
45	Dielectric constant of a highly polarizable atomic fluid: the clausiusâ€"mossotti versus the onsager relation. Molecular Physics, 2004, 102, 783-788.	0.8	7
46	Computing the electrostatic free-energy of complex molecules: The variational Coulomb field approximation. Journal of Chemical Physics, 2003, 119, 3516-3528.	1.2	23
47	Molecular simulation of a hydrated electron at different thermodynamic state points. Journal of Chemical Physics, 2003, 118, 9689-9696.	1.2	66
48	Density functional theory of solvation in a polar solvent: Extracting the functional from homogeneous solvent simulations. Physical Review E, 2002, 66, 031206.	0.8	63
49	Electrostatics on particles: Phenomenological and orientational density functional theory approach. Journal of Chemical Physics, 2002, 117, 541-556.	1.2	31
50	Analytical investigations of an electronâ€"water molecule pseudopotential. II. Development of a new pair potential and molecular dynamics simulations. Journal of Chemical Physics, 2002, 117, 6186-6195.	1.2	147
51	A dielectric continuum molecular dynamics method. Journal of Chemical Physics, 2001, 114, 4377.	1.2	57
52	Analytical investigations of an electronâ€"water molecule pseudopotential. I. Exact calculations on a model system. Journal of Chemical Physics, 2001, 114, 7805-7815.	1.2	54
53	Transport and spectroscopy of the hydrated proton: A molecular dynamics study. Journal of Chemical Physics, 1999, 111, 4251-4266.	1.2	261
54	An extended empirical valence bond model for describing proton transfer in H+(H2O)n clusters and liquid water. Chemical Physics Letters, 1998, 284, 71-77.	1.2	173

#	Article	IF	Citations
55	Quantum Dynamics of an Excess Proton in Water Using an Extended Empirical Valence-Bond Hamiltonian. Journal of Physical Chemistry B, 1998, 102, 4261-4264.	1.2	159
56	A quantum multi-mode molecular dynamics approach to the vibrational spectroscopy of solvated hydrogen-bonded complexes. Chemical Physics Letters, 1997, 271, 232-240.	1.2	22
57	Reaction pathways in the photodetachment of an electron from aqueous chloride: A quantum molecular dynamics study. Journal of Chemical Physics, 1996, 104, 9027-9039.	1.2	105
58	Quantum adiabatic umbrella sampling: The excited state free energy surface of an electronâ€atom pair in solution. Journal of Chemical Physics, 1996, 104, 4776-4783.	1.2	58
59	Ultrafast spectroscopy of the aqueous chloride ion studied by quantum molecular dynamics simulations. Journal of Physics Condensed Matter, 1996, 8, 9389-9395.	0.7	6
60	A semiempirical quantum polarization model for water. Chemical Physics Letters, 1995, 238, 187-192.	1.2	31
61	Molecular dynamics simulation of an excess charge in water using mobile Gaussian orbitals. Journal of Chemical Physics, 1995, 103, 2642-2655.	1.2	190
62	Proton transfer in hydrogenâ€bonded acidâ€“base complexes in polar solvents. Journal of Chemical Physics, 1995, 102, 2487-2505.	1.2	202
63	Excited states of a hydrated electron and aqueous chloride by computer simulation. Chemical Physics Letters, 1994, 230, 405-413.	1.2	58
64	Density functional theory applied to proton-transfer systems. A numerical test. Chemical Physics Letters, 1993, 208, 364-368.	1.2	89
65	Dynamical theory of proton tunneling transfer rates in solution: general formulation. Chemical Physics, 1993, 170, 315-346.	0.9	228
66	Molecularâ€dynamics simulation for a model nonadiabatic proton transfer reaction in solution. Journal of Chemical Physics, 1991, 94, 3619-3628.	1.2	323
67	A class of collision processes with memory and application to simple chemical reactions in a solvent. Journal of Statistical Physics, 1986, 45, 319-347.	0.5	3