

# Daniel Borgis

## List of Publications by Year in descending order

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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	Molecular dynamics simulation for a model nonadiabatic proton transfer reaction in solution. <i>Journal of Chemical Physics</i> , 1991, 94, 3619-3628.	1.2	323
2	Transport and spectroscopy of the hydrated proton: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1999, 111, 4251-4266.	1.2	261
3	Dynamical theory of proton tunneling transfer rates in solution: general formulation. <i>Chemical Physics</i> , 1993, 170, 315-346.	0.9	228
4	Proton transfer in hydrogen-bonded acid-base complexes in polar solvents. <i>Journal of Chemical Physics</i> , 1995, 102, 2487-2505.	1.2	202
5	Molecular dynamics simulation of an excess charge in water using mobile Gaussian orbitals. <i>Journal of Chemical Physics</i> , 1995, 103, 2642-2655.	1.2	190
6	An extended empirical valence bond model for describing proton transfer in $H+(H_2O)_n$ clusters and liquid water. <i>Chemical Physics Letters</i> , 1998, 284, 71-77.	1.2	173
7	Quantum Dynamics of an Excess Proton in Water Using an Extended Empirical Valence-Bond Hamiltonian. <i>Journal of Physical Chemistry B</i> , 1998, 102, 4261-4264.	1.2	159
8	Analytical investigations of an electron-water molecule pseudopotential. II. Development of a new pair potential and molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2002, 117, 6186-6195.	1.2	147
9	Reaction pathways in the photodetachment of an electron from aqueous chloride: A quantum molecular dynamics study. <i>Journal of Chemical Physics</i> , 1996, 104, 9027-9039.	1.2	105
10	A Coarse-Grained Protein-Protein Potential Derived from an All-Atom Force Field. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9390-9399.	1.2	92
11	Density functional theory applied to proton-transfer systems. A numerical test. <i>Chemical Physics Letters</i> , 1993, 208, 364-368.	1.2	89
12	Molecular density functional theory of solvation: From polar solvents to water. <i>Journal of Chemical Physics</i> , 2011, 134, 194102.	1.2	86
13	Molecular Density Functional Theory of Water. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 619-624.	2.1	76
14	Density Functional Theory of Solvation and Its Relation to Implicit Solvent Models. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6754-6763.	1.2	74
15	Fast Computation of Solvation Free Energies with Molecular Density Functional Theory: Thermodynamic-Ensemble Partial Molar Volume Corrections. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1935-1942.	2.1	67
16	Solvation free-energy pressure corrections in the three dimensional reference interaction site model. <i>Journal of Chemical Physics</i> , 2015, 143, 184116.	1.2	67
17	Molecular simulation of a hydrated electron at different thermodynamic state points. <i>Journal of Chemical Physics</i> , 2003, 118, 9689-9696.	1.2	66
18	Density functional theory of solvation in a polar solvent: Extracting the functional from homogeneous solvent simulations. <i>Physical Review E</i> , 2002, 66, 031206.	0.8	63

#	ARTICLE	IF	CITATIONS
19	Excited states of a hydrated electron and aqueous chloride by computer simulation. <i>Chemical Physics Letters</i> , 1994, 230, 405-413.	1.2	58
20	Quantum adiabatic umbrella sampling: The excited state free energy surface of an electron-atom pair in solution. <i>Journal of Chemical Physics</i> , 1996, 104, 4776-4783.	1.2	58
21	A dielectric continuum molecular dynamics method. <i>Journal of Chemical Physics</i> , 2001, 114, 4377.	1.2	57
22	Analytical investigations of an electron-water molecule pseudopotential. I. Exact calculations on a model system. <i>Journal of Chemical Physics</i> , 2001, 114, 7805-7815.	1.2	54
23	Classical density functional theory of solvation in molecular solvents: Angular grid implementation. <i>Chemical Physics Letters</i> , 2009, 474, 366-370.	1.2	49
24	Modeling Protein-Protein Recognition in Solution Using the Coarse-Grained Force Field SCORPION. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 803-813.	2.3	47
25	Hopping along hydrogen bonds. <i>Nature Chemistry</i> , 2012, 4, 432-433.	6.6	46
26	Combining a polarizable force field and a coarse-grained polarizable solvent model: Application to long dynamics simulations of bovine pancreatic trypsin inhibitor. <i>Journal of Computational Chemistry</i> , 2008, 29, 1707-1724.	1.5	42
27	A polarizable coarse-grained water model for coarse-grained proteins simulations. <i>Chemical Physics Letters</i> , 2009, 468, 79-82.	1.2	42
28	Molecular Density Functional Theory: Application to Solvation and Electron-Transfer Thermodynamics in Polar Solvents. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2504-2512.	1.2	42
29	Extension of Marcus Picture for Electron Transfer Reactions with Large Solvation Changes. <i>Journal of the American Chemical Society</i> , 2012, 134, 2067-2074.	6.6	42
30	Scalar fundamental measure theory for hard spheres in three dimensions: Application to hydrophobic solvation. <i>Journal of Chemical Physics</i> , 2012, 137, 034115.	1.2	42
31	Computation of pair distribution functions and three-dimensional densities with a reduced variance principle. <i>Molecular Physics</i> , 2013, 111, 3486-3492.	0.8	39
32	Direct correlation functions and the density functional theory of polar solvents. <i>Chemical Physics</i> , 2005, 319, 261-272.	0.9	38
33	Molecular density functional theory of water describing hydrophobicity at short and long length scales. <i>Journal of Chemical Physics</i> , 2013, 139, 154101.	1.2	37
34	Computing Wigner distributions and time correlation functions using the quantum thermal bath method: application to proton transfer spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 12591.	1.3	32
35	A semiempirical quantum polarization model for water. <i>Chemical Physics Letters</i> , 1995, 238, 187-192.	1.2	31
36	Electrostatics on particles: Phenomenological and orientational density functional theory approach. <i>Journal of Chemical Physics</i> , 2002, 117, 541-556.	1.2	31

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37	Study of a water-graphene capacitor with molecular density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 124111.	1.2	31
38	Nuclear quantum effects on the nonadiabatic decay mechanism of an excited hydrated electron. <i>Journal of Chemical Physics</i> , 2007, 127, 174508.	1.2	29
39	Efficient molecular density functional theory using generalized spherical harmonics expansions. <i>Journal of Chemical Physics</i> , 2017, 147, 094107.	1.2	29
40	Combining a polarizable force field and a coarse-grained polarizable solvent model. II. Accounting for hydrophobic effects. <i>Journal of Computational Chemistry</i> , 2011, 32, 2664-2678.	1.5	28
41	Molecular density functional theory for water with liquid-gas coexistence and correct pressure. <i>Journal of Chemical Physics</i> , 2015, 142, 154112.	1.2	26
42	A molecular density functional theory approach to electron transfer reactions. <i>Chemical Science</i> , 2019, 10, 2130-2143.	3.7	24
43	Computing the electrostatic free-energy of complex molecules: The variational Coulomb field approximation. <i>Journal of Chemical Physics</i> , 2003, 119, 3516-3528.	1.2	23
44	Solvation of complex surfaces via molecular density functional theory. <i>Journal of Chemical Physics</i> , 2012, 137, 224107.	1.2	23
45	A quantum multi-mode molecular dynamics approach to the vibrational spectroscopy of solvated hydrogen-bonded complexes. <i>Chemical Physics Letters</i> , 1997, 271, 232-240.	1.2	22
46	A semi-implicit solvent model for the simulation of peptides and proteins. <i>Journal of Computational Chemistry</i> , 2004, 25, 1015-1029.	1.5	22
47	Screened Coulombic Orientational Correlations in Dilute Aqueous Electrolytes. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1985-1989.	2.1	22
48	Hydration free energies and solvation structures with molecular density functional theory in the hypernetted chain approximation. <i>Journal of Chemical Physics</i> , 2020, 152, 064110.	1.2	21
49	Particle-Based Implicit Solvent Model for Biosimulations: Application to Proteins and Nucleic Acids Hydration. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1646-1656.	2.3	20
50	Tackling Solvent Effects by Coupling Electronic and Molecular Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7123-7134.	2.3	19
51	A multiscale coarse-grained polarizable solvent model for handling long tail bulk electrostatics. <i>Journal of Computational Chemistry</i> , 2013, 34, 1112-1124.	1.5	17
52	Generating approximate Wigner distributions using Gaussian phase packets propagation in imaginary time. <i>Chemical Physics Letters</i> , 2006, 423, 390-394.	1.2	15
53	Molecular density functional theory of water including density polarization coupling. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 244005.	0.7	15
54	Electronic Excited State Lifetimes of Anionic Water Clusters: Dependence on Charge Solvation Motif. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2304-2309.	2.1	15

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55	What Does Second-Harmonic Scattering Measure in Diluted Electrolytes?. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3698-3702.	2.1	15
56	Simple Parameter-Free Bridge Functionals for Molecular Density Functional Theory. Application to Hydrophobic Solvation. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6885-6893.	1.2	13
57	Computing three-dimensional densities from force densities improves statistical efficiency. <i>Journal of Chemical Physics</i> , 2019, 151, 064124.	1.2	12
58	Hydration of clays at the molecular scale: the promising perspective of classical density functional theory. <i>Molecular Physics</i> , 2014, 112, 1320-1329.	0.8	11
59	A dielectric continuum model of solvation for complex solutes. <i>Computer Physics Communications</i> , 2005, 169, 69-74.	3.0	9
60	Coarse-Graining the Accessible Surface and the Electrostatics of Proteins for Protein-Protein Interactions. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1867-1876.	2.3	9
61	Accurate prediction of hydration free energies and solvation structures using molecular density functional theory with a simple bridge functional. <i>Journal of Chemical Physics</i> , 2021, 155, 024117.	1.2	9
62	Introduction to Classical Density Functional Theory by a Computational Experiment. <i>Journal of Chemical Education</i> , 2014, 91, 2112-2115.	1.1	8
63	Dielectric constant of a highly polarizable atomic fluid: the clausius-mossotti versus the onsager relation. <i>Molecular Physics</i> , 2004, 102, 783-788.	0.8	7
64	Ultrafast spectroscopy of the aqueous chloride ion studied by quantum molecular dynamics simulations. <i>Journal of Physics Condensed Matter</i> , 1996, 8, 9389-9395.	0.7	6
65	Predicting Hydration Free Energies of the FreeSolv Database of Drug-like Molecules with Molecular Density Functional Theory. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3558-3565.	2.5	6
66	Quantifying Fluctuations of Average Solvent Environments for Embedding Calculations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1072-1088.	2.3	4
67	A class of collision processes with memory and application to simple chemical reactions in a solvent. <i>Journal of Statistical Physics</i> , 1986, 45, 319-347.	0.5	3