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List of Publications by Year
in descending order

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91 papers	9,426 citations	50276 46 h-index	42399 92 g-index
94 all docs	94 docs citations	94 times ranked	6528 citing authors

#	Article	IF	Citations
1	Accurate Free Energies for Complex Condensed-Phase Reactions Using an Artificial Neural Network Corrected DFTB/MM Methodology. Journal of Chemical Theory and Computation, 2022, 18, 1213-1226.	5.3	18
2	Unravelling the mechanism of glucose binding in a protein-based fluorescence probe: molecular dynamics simulation with a tailor-made charge model. Physical Chemistry Chemical Physics, 2022, 24, 2441-2453.	2.8	2
3	Understanding excited state properties of host materials in OLEDs: simulation of absorption spectrum of amorphous 4,4-bis(carbazol-9-yl)-2,2-biphenyl (CBP). Physical Chemistry Chemical Physics, 2022, , .	2.8	2
4	Efficient Surface Hopping Approach for Modeling Charge Transport in Organic Semiconductors. Journal of Chemical Theory and Computation, 2022, 18, 1264-1274.	5.3	4
5	Interplay of structural dynamics and electronic effects in an engineered assembly of pentacene in a metalâ€“organic framework. Chemical Science, 2021, 12, 4477-4483.	7.4	18
6	Analytical Time-Dependent Long-Range Corrected Density Functional Tight Binding (TD-LC-DFTB) Gradients in DFTB+: Implementation and Benchmark for Excited-State Geometries and Transition Energies. Journal of Chemical Theory and Computation, 2021, 17, 2266-2282.	5.3	10
7	Geometry dependence of excitonic couplings and the consequences for configurationâ€space sampling. Journal of Computational Chemistry, 2021, 42, 1402-1418.	3.3	5
8	O to bR transition in bacteriorhodopsin occurs through a proton hole mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	5
9	Multiscale QM/MM molecular dynamics simulations of the trimeric major light-harvesting complex II. Physical Chemistry Chemical Physics, 2021, 23, 7407-7417.	2.8	24
10	HAB79: A New Molecular Dataset for Benchmarking DFT and DFTB Electronic Couplings Against High-Level Ab-initio Calculations. Journal of Chemical Physics, 2021, 155, 234115.	3.0	14
11	Electrostatic interactions contribute to the control of intramolecular thiolâ€“disulfide isomerization in a protein. Physical Chemistry Chemical Physics, 2021, 23, 26366-26375.	2.8	6
12	DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. Journal of Physical Chemistry Letters, 2020, 11, 8660-8667.	4.6	34
13	Charge and Exciton Transfer Simulations Using Machine-Learned Hamiltonians. Journal of Chemical Theory and Computation, 2020, 16, 4061-4070.	5.3	30
14	Performance of Mixed Quantum-Classical Approaches on Modeling the Crossover from Hopping to Bandlike Charge Transport in Organic Semiconductors. Journal of Chemical Theory and Computation, 2020, 16, 2071-2084.	5.3	21
15	Benchmark and performance of long-range corrected time-dependent density functional tight binding (LC-TD-DFTB) on rhodopsins and light-harvesting complexes. Physical Chemistry Chemical Physics, 2020, 22, 10500-10518.	2.8	36
16	Improvement of dâ€“d interactions in density functional tight binding for transition metal ions with a ligand field model: assessment of a DFTB3+U model on nickel coordination compounds. Physical Chemistry Chemical Physics, 2020, 22, 27084-27095.	2.8	3
17	Origin of the Solvatochromism in Organic Fluorophores with Flexible Side Chains: A Case Study of Flugi-2. Journal of Physical Chemistry A, 2019, 123, 4581-4587.	2.5	3
18	Exploring the applicability of density functional tight binding to transition metal ions. Parameterization for nickel with the spinâ€polarized DFTB3 model. Journal of Computational Chemistry, 2019, 40, 400-413.	3.3	13

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19	Parametrization and Benchmark of Long-Range Corrected DFTB2 for Organic Molecules. Journal of Chemical Theory and Computation, 2018, 14, 115-125.	5.3	60
20	â€œsiRNA traffic lightsâ€• arabino-configured 2â€²-anchors for fluorescent dyes are key for dual color readout in cell imaging. Organic and Biomolecular Chemistry, 2018, 16, 3726-3731.	2.8	4
21	Best of Two Worlds? How MD Simulations of Amphiphilic Helical Peptides in Membranes Can Complement Data from Oriented Solid-State NMR. Journal of Chemical Theory and Computation, 2018, 14, 6002-6014.	5.3	12
22	On the mechanism of spontaneous thiolâ€“disulfide exchange in proteins. Physical Chemistry Chemical Physics, 2018, 20, 16222-16230.	2.8	22
23	Coupled-perturbed DFTB-QM/MM metadynamics: Application to proton-coupled electron transfer. Journal of Chemical Physics, 2018, 149, 072328.	3.0	14
24	Molecular Insights into Variable Electron Transfer in Amphibian Cryptochrome. Biophysical Journal, 2018, 114, 2563-2572.	0.5	17
25	Time-Dependent Extension of the Long-Range Corrected Density Functional Based Tight-Binding Method. Journal of Chemical Theory and Computation, 2017, 13, 1737-1747.	5.3	67
26	Polaron Effects on Charge Transport through Molecular Wires: A Multiscale Approach. Journal of Chemical Theory and Computation, 2017, 13, 286-296.	5.3	16
27	Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules. Journal of Computational Chemistry, 2017, 38, 2171-2185.	3.3	39
28	Reaction dynamics of the chimeric channelrhodopsin C1C2. Scientific Reports, 2017, 7, 7217.	3.3	48
29	Simulation of Temperature-Dependent Charge Transport in Organic Semiconductors with Various Degrees of Disorder. Journal of Chemical Theory and Computation, 2016, 12, 3087-3096.	5.3	27
30	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. Chemical Reviews, 2016, 116, 5301-5337.	47.7	312
31	Electronic Coupling Calculations for Bridge-Mediated Charge Transfer Using Constrained Density Functional Theory (CDFT) and Effective Hamiltonian Approaches at the Density Functional Theory (DFT) and Fragment-Orbital Density Functional Tight Binding (FODFTB) Level. Journal of Chemical Theory and Computation, 2016, 12, 4793-4805.	5.3	46
32	Simulation of Singlet Exciton Diffusion in Bulk Organic Materials. Journal of Chemical Theory and Computation, 2016, 12, 4209-4221.	5.3	22
33	Active site structure and absorption spectrum of channelrhodopsin-2 wild-type and C128T mutant. Chemical Science, 2016, 7, 3879-3891.	7.4	40
34	Relation between Dephasing Time and Energy Gap Fluctuations in Biomolecular Systems. Journal of Physical Chemistry Letters, 2016, 7, 1102-1108.	4.6	10
35	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. Journal of Chemical Physics, 2015, 143, 084123.	3.0	47
36	Molecular Dynamics Investigation of gluazo, a Photo-Switchable Ligand for the Glutamate Receptor GluK2. PLoS ONE, 2015, 10, e0135399.	2.5	8

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37	Electronic couplings for molecular charge transfer: benchmarking CDFT, FODFT and FODFTB against high-level ab initio calculations. II. Physical Chemistry Chemical Physics, 2015, 17, 14342-14354.	2.8	119
38	QM/QM Approach to Model Energy Disorder in Amorphous Organic Semiconductors. Journal of Chemical Theory and Computation, 2015, 11, 560-567.	5.3	40
39	Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. Journal of Chemical Theory and Computation, 2015, 11, 4992-5001.	5.3	42
40	Multi-Scale Approach to Non-Adiabatic Charge Transport in High-Mobility Organic Semiconductors. Journal of Chemical Theory and Computation, 2015, 11, 5068-5082.	5.3	53
41	DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters. Journal of Chemical Theory and Computation, 2015, 11, 4205-4219.	5.3	30
42	Parameterization of the DFTB3 Method for Br, Ca, Cl, F, I, K, and Na in Organic and Biological Systems. Journal of Chemical Theory and Computation, 2015, 11, 332-342.	5.3	227
43	Mechanism by which Untwisting of Retinal Leads to Productive Bacteriorhodopsin Photocycle States. Journal of Physical Chemistry B, 2015, 119, 2229-2240.	2.6	12
44	Parametrization of DFTB3/3OB for Magnesium and Zinc for Chemical and Biological Applications. Journal of Physical Chemistry B, 2015, 119, 1062-1082.	2.6	138
45	Parameterization of DFTB3/3OB for Sulfur and Phosphorus for Chemical and Biological Applications. Journal of Chemical Theory and Computation, 2014, 10, 1518-1537.	5.3	275
46	Density functional tight binding. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120483.	3.4	256
47	Electronic couplings for molecular charge transfer: Benchmarking CDFT, FODFT, and FODFTB against high-level ab initio calculations. Journal of Chemical Physics, 2014, 140, 104105.	3.0	175
48	Density functional tight binding: values of semi-empirical methods in an ab initio era. Physical Chemistry Chemical Physics, 2014, 16, 14368-14377.	2.8	125
49	Size-Consistent Multipartitioning QM/MM: A Stable and Efficient Adaptive QM/MM Method. Journal of Chemical Theory and Computation, 2014, 10, 4242-4252.	5.3	55
50	Density functional tight binding: application to organic and biological molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 49-61.	14.6	157
51	Ligand Photo-Isomerization Triggers Conformational Changes in iGluR2 Ligand Binding Domain. PLoS ONE, 2014, 9, e92716.	2.5	8
52	Towards an Understanding of Channelrhodopsin Function: Simulations Lead to Novel Insights of the Channel Mechanism. Journal of Molecular Biology, 2013, 425, 1795-1814.	4.2	62
53	Parametrization and Benchmark of DFTB3 for Organic Molecules. Journal of Chemical Theory and Computation, 2013, 9, 338-354.	5.3	743
54	Modeling charge transport in DNA using multiâ€scale methods. Physica Status Solidi (B): Basic Research, 2013, 250, 2277-2287.	1.5	26

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55	Computational Study of Synthetic Agonist Ligands of Ionotropic Glutamate Receptors. PLoS ONE, 2013, 8, e58774.	2.5	11
56	Parametrization of the SCC-DFTB Method for Halogens. Journal of Chemical Theory and Computation, 2013, 9, 2939-2949.	5.3	54
57	A hybrid approach to simulation of electron transfer in complex molecular systems. Journal of the Royal Society Interface, 2013, 10, 20130415.	3.4	72
58	A Modified QM/MM Hamiltonian with the Self-Consistent-Charge Density-Functional-Tight-Binding Theory for Highly Charged QM Regions. Journal of Chemical Theory and Computation, 2012, 8, 4293-4304.	5.3	30
59	Extended Polarization in Third-Order SCC-DFTB from Chemical-Potential Equalization. Journal of Physical Chemistry A, 2012, 116, 9131-9141.	2.5	42
60	Improved Electronic Properties from Third-Order SCC-DFTB with Cost Efficient Post-SCF Extensions. Journal of Physical Chemistry A, 2012, 116, 11927-11937.	2.5	16
61	Application of the SCC-DFTB Method to Neutral and Protonated Water Clusters and Bulk Water. Journal of Physical Chemistry B, 2011, 115, 6790-6805.	2.6	81
62	Color Tuning in Binding Pocket Models of the Chlamydomonas-Type Channelrhodopsins. Journal of Physical Chemistry B, 2011, 115, 15119-15128.	2.6	28
63	DFTB3: Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method (SCC-DFTB). Journal of Chemical Theory and Computation, 2011, 7, 931-948.	5.3	828
64	Mechanism of a proton pump analyzed with computer simulations. Theoretical Chemistry Accounts, 2010, 125, 353-363.	1.4	15
65	The Protonation State of Glu181 in Rhodopsin Revisited: Interpretation of Experimental Data on the Basis of QM/MM Calculations. Journal of Physical Chemistry B, 2010, 114, 11338-11352.	2.6	50
66	Coarse-Grained Time-Dependent Density Functional Simulation of Charge Transfer in Complex Systems: Application to Hole Transfer in DNA. Journal of Physical Chemistry B, 2010, 114, 11221-11240.	2.6	79
67	Combined density functional theory and Landauer approach for hole transfer in DNA along classical molecular dynamics trajectories. Journal of Chemical Physics, 2009, 130, 215104.	3.0	78
68	Automatized Parametrization of SCC-DFTB Repulsive Potentials: Application to Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 11866-11881.	2.5	69
69	Efficient Calculation of Charge-Transfer Matrix Elements for Hole Transfer in DNA. Journal of Physical Chemistry B, 2008, 112, 7937-7947.	2.6	150
70	Effect of Polarization on the Opsin Shift in Rhodopsins. 1. A Combined QM/QM/MM Model for Bacteriorhodopsin and Pharaonis Sensory Rhodopsin II. Journal of Physical Chemistry B, 2008, 112, 11462-11467.	2.6	62
71	Description of Phosphate Hydrolysis Reactions with the Self-Consistent-Charge Density-Functional-Tight-Binding (SCC-DFTB) Theory. 1. Parameterization. Journal of Chemical Theory and Computation, 2008, 4, 2067-2084.	5.3	87
72	Effect of Polarization on the Opsin Shift in Rhodopsins. 2. Empirical Polarization Models for Proteins. Journal of Physical Chemistry B, 2008, 112, 11468-11478.	2.6	49

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73	Parameter Calibration of Transition-Metal Elements for the Spin-Polarized Self-Consistent-Charge Density-Functional Tight-Binding (DFTB) Method:â€‰ Sc, Ti, Fe, Co, and Ni. Journal of Chemical Theory and Computation, 2007, 3, 1349-1367.	5.3	208
74	Implementation of the SCC-DFTB Method for Hybrid QM/MM Simulations within the Amber Molecular Dynamics Packageâ€. Journal of Physical Chemistry A, 2007, 111, 5655-5664.	2.5	213
75	Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method:â€‰ Third-Order Expansion of the Density Functional Theory Total Energy and Introduction of a Modified Effective Coulomb Interaction. Journal of Physical Chemistry A, 2007, 111, 10861-10873.	2.5	265
76	Simulating Water with the Self-Consistent-Charge Density Functional Tight Binding Method:Â From Molecular Clusters to the Liquid Stateâ€. Journal of Physical Chemistry A, 2007, 111, 5685-5691.	2.5	79
77	Color Tuning in Rhodopsins:Â The Mechanism for the Spectral Shift between Bacteriorhodopsin and Sensory Rhodopsin II. Journal of the American Chemical Society, 2006, 128, 10808-10818.	13.7	196
78	Development of Effective Quantum Mechanical/Molecular Mechanical (QM/MM) Methods for Complex Biological Processes. Journal of Physical Chemistry B, 2006, 110, 6458-6469.	2.6	290
79	Computational photochemistry of retinal proteins. Journal of Computer-Aided Molecular Design, 2006, 20, 511-518.	2.9	50
80	Validation of the density-functional based tight-binding approximation method for the calculation of reaction energies and other data. Journal of Chemical Physics, 2005, 122, 114110.	3.0	140
81	Quantum Chemical Molecular Dynamics Model Study of Fullerene Formation from Open-Ended Carbon Nanotubesâ€. Journal of Physical Chemistry A, 2004, 108, 3182-3194.	2.5	43
82	Modeling zinc in biomolecules with the self consistent charge-density functional tight binding (SCC-DFTB) method: Applications to structural and energetic analysis. Journal of Computational Chemistry, 2003, 24, 565-581.	3.3	150
83	An approximate DFT method for QM/MM simulations of biological structures and processes. Computational and Theoretical Chemistry, 2003, 632, 29-41.	1.5	172
84	Comparison of a QM/MM force field and molecular mechanics force fields in simulations of alanine and glycine â€œdipeptidesâ€•(Ace-Ala-Nme and Ace-Gly-Nme) in water in relation to the problem of modeling the unfolded peptide backbone in solution. Proteins: Structure, Function and Bioinformatics, 2003, 50, 451-463.	2.6	250
85	From C2Molecules to Self-Assembled Fullerenes in Quantum Chemical Molecular Dynamics. Nano Letters, 2003, 3, 1657-1664.	9.1	87
86	Formation of Fullerene Molecules from Carbon Nanotubes:Â A Quantum Chemical Molecular Dynamics Study. Nano Letters, 2003, 3, 465-470.	9.1	50
87	A QM/MM Implementation of the Self-Consistent Charge Density Functional Tight Binding (SCC-DFTB) Method. Journal of Physical Chemistry B, 2001, 105, 569-585.	2.6	568
88	Energetics and structure of glycine and alanine based model peptides: Approximate SCC-DFTB, AM1 and PM3 methods in comparison with DFT, HF and MP2 calculations. Chemical Physics, 2001, 263, 203-219.	1.9	132
89	Quantum mechanics simulation of protein dynamics on long timescale. Proteins: Structure, Function and Bioinformatics, 2001, 44, 484-489.	2.6	140
90	Hydrogen bonding and stacking interactions of nucleic acid base pairs: A density-functional-theory based treatment. Journal of Chemical Physics, 2001, 114, 5149-5155.	3.0	978

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91	Hydrogen Storage in Single-Walled and Multi-Walled Carbon Nanotubes. Materials Research Society Symposia Proceedings, 1999, 593, 187.	0.1	1