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List of Publications by Year
in descending order

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91 papers	9,426 citations	50273 46 h-index	42393 92 g-index
94 all docs	94 docs citations	94 times ranked	6528 citing authors

#	Article	IF	Citations
1	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
2	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
3	Parametrization and Benchmark of DFTB3 for Organic Molecules. Journal of Chemical Theory and Computation, 2013, 9, 338-354.	5.3	743
4	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
5	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. Chemical Reviews, 2016, 116, 5301-5337.	47.7	312
6	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
7	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
8	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
9	Density functional tight binding. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120483.	3.4	256
10	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
11	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
12	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
13	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
14	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
15	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
16	An approximate DFT method for QM/MM simulations of biological structures and processes. Computational and Theoretical Chemistry, 2003, 632, 29-41.	1.5	172
17	Density functional tight binding: application to organic and biological molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 49-61.	14.6	157
18	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

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19	Efficient Calculation of Charge-Transfer Matrix Elements for Hole Transfer in DNA. Journal of Physical Chemistry B, 2008, 112, 7937-7947.	2.6	150
20	Quantum mechanics simulation of protein dynamics on long timescale. Proteins: Structure, Function and Bioinformatics, 2001, 44, 484-489.	2.6	140
21	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
22	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
23	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
24	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
25	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
26	From C2Molecules to Self-Assembled Fullerenes in Quantum Chemical Molecular Dynamics. Nano Letters, 2003, 3, 1657-1664.	9.1	87
27	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
28	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
29	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
30	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
31	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
32	A hybrid approach to simulation of electron transfer in complex molecular systems. Journal of the Royal Society Interface, 2013, 10, 20130415.	3.4	72
33	Automatized Parametrization of SCC-DFTB Repulsive Potentials: Application to Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 11866-11881.	2.5	69
34	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
35	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
36	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

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37	Parametrization and Benchmark of Long-Range Corrected DFTB2 for Organic Molecules. Journal of Chemical Theory and Computation, 2018, 14, 115-125.	5.3	60
38	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
39	Parametrization of the SCC-DFTB Method for Halogens. Journal of Chemical Theory and Computation, 2013, 9, 2939-2949.	5.3	54
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	Formation of Fullerene Molecules from Carbon Nanotubes:Â A Quantum Chemical Molecular Dynamics Study. Nano Letters, 2003, 3, 465-470.	9.1	50
42	Computational photochemistry of retinal proteins. Journal of Computer-Aided Molecular Design, 2006, 20, 511-518.	2.9	50
43	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
44	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
45	Reaction dynamics of the chimeric channelrhodopsin C1C2. Scientific Reports, 2017, 7, 7217.	3.3	48
46	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. Journal of Chemical Physics, 2015, 143, 084123.	3.0	47
47	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
48	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
49	Extended Polarization in Third-Order SCC-DFTB from Chemical-Potential Equalization. Journal of Physical Chemistry A, 2012, 116, 9131-9141.	2.5	42
50	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
51	QM/QM Approach to Model Energy Disorder in Amorphous Organic Semiconductors. Journal of Chemical Theory and Computation, 2015, 11, 560-567.	5.3	40
52	Active site structure and absorption spectrum of channelrhodopsin-2 wild-type and C128T mutant. Chemical Science, 2016, 7, 3879-3891.	7.4	40
53	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
54	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

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55	DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. Journal of Physical Chemistry Letters, 2020, 11, 8660-8667.	4.6	34
56	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
57	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
58	Charge and Exciton Transfer Simulations Using Machine-Learned Hamiltonians. Journal of Chemical Theory and Computation, 2020, 16, 4061-4070.	5.3	30
59	Color Tuning in Binding Pocket Models of the Chlamydomonas-Type Channelrhodopsins. Journal of Physical Chemistry B, 2011, 115, 15119-15128.	2.6	28
60	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
61	Modeling charge transport in DNA using multiâ€scale methods. Physica Status Solidi (B): Basic Research, 2013, 250, 2277-2287.	1.5	26
62	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
63	Simulation of Singlet Exciton Diffusion in Bulk Organic Materials. Journal of Chemical Theory and Computation, 2016, 12, 4209-4221.	5.3	22
64	On the mechanism of spontaneous thiolâ€“disulfide exchange in proteins. Physical Chemistry Chemical Physics, 2018, 20, 16222-16230.	2.8	22
65	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
66	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
67	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
68	Molecular Insights into Variable Electron Transfer in Amphibian Cryptochrome. Biophysical Journal, 2018, 114, 2563-2572.	0.5	17
69	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
70	Polaron Effects on Charge Transport through Molecular Wires: A Multiscale Approach. Journal of Chemical Theory and Computation, 2017, 13, 286-296.	5.3	16
71	Mechanism of a proton pump analyzed with computer simulations. Theoretical Chemistry Accounts, 2010, 125, 353-363.	1.4	15
72	Coupled-perturbed DFTB-QM/MM metadynamics: Application to proton-coupled electron transfer. Journal of Chemical Physics, 2018, 149, 072328.	3.0	14

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73	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
74	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
75	Mechanism by which Untwisting of Retinal Leads to Productive Bacteriorhodopsin Photocycle States. Journal of Physical Chemistry B, 2015, 119, 2229-2240.	2.6	12
76	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
77	Computational Study of Synthetic Agonist Ligands of Ionotropic Glutamate Receptors. PLoS ONE, 2013, 8, e58774.	2.5	11
78	Relation between Dephasing Time and Energy Gap Fluctuations in Biomolecular Systems. Journal of Physical Chemistry Letters, 2016, 7, 1102-1108.	4.6	10
79	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
80	Molecular Dynamics Investigation of gluazo, a Photo-Switchable Ligand for the Glutamate Receptor GluK2. PLoS ONE, 2015, 10, e0135399.	2.5	8
81	Ligand Photo-Isomerization Triggers Conformational Changes in iGluR2 Ligand Binding Domain. PLoS ONE, 2014, 9, e92716.	2.5	8
82	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
83	Geometry dependence of excitonic couplings and the consequences for configurationâ€space sampling. Journal of Computational Chemistry, 2021, 42, 1402-1418.	3.3	5
84	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
85	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
86	Efficient Surface Hopping Approach for Modeling Charge Transport in Organic Semiconductors. Journal of Chemical Theory and Computation, 2022, 18, 1264-1274.	5.3	4
87	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
88	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
89	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
90	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

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