Marcus Elstner

List of Publications by Citations

88 papers	7,814 citations	43 h-index	88 g-index
94 ext. papers	8,673 ext. citations	5.5 avg, IF	6.17 L-index

#	Paper	IF	Citations
88	Hydrogen bonding and stacking interactions of nucleic acid base pairs: A density-functional-theory based treatment. *Journal of Chemical Physics*, **2001**, 114, 5149-5155	3.9	925
87	DFTB3: Extension of the self-consistent-charge density-functional tight-binding method (SCC-DFTB). *Journal of Chemical Theory and Computation*, **2012**, 7, 931-948	6.4	620
86	Parametrization and Benchmark of DFTB3 for Organic Molecules. *Journal of Chemical Theory and Computation*, **2013**, 9, 338-54	6.4	524
85	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	3.4	523
84	Development of effective quantum mechanical/molecular mechanical (QM/MM) methods for complex biological processes. *Journal of Physical Chemistry B*, **2006**, 110, 6458-69	3.4	274
83	Comparison of a QM/MM force field and molecular mechanics force fields in simulations of alanine and glycine "dipeptides" (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, 451-63	4.2	230
82	Extension of the self-consistent-charge density-functional tight-binding method: 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, 10861-73	2.8	221
81	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. *Chemical Reviews*, **2016**, 116, 5301-37	68.1	210
80	Parameterization of DFTB3/3OB for Sulfur and Phosphorus for Chemical and Biological Applications. *Journal of Chemical Theory and Computation*, **2014**, 10, 1518-1537	6.4	195
79	Implementation of the SCC-DFTB method for hybrid QM/MM simulations within the amber molecular dynamics package. *Journal of Physical Chemistry A*, **2007**, 111, 5655-64	2.8	183
78	Density functional tight binding. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2014**, 372, 20120483	3	182
77	Color tuning in rhodopsins: the mechanism for the spectral shift between bacteriorhodopsin and sensory rhodopsin II. *Journal of the American Chemical Society*, **2006**, 128, 10808-18	16.4	179
76	Parameter Calibration of Transition-Metal Elements for the Spin-Polarized Self-Consistent-Charge Density-Functional Tight-Binding (DFTB) Method: Sc, Ti, Fe, Co, and Ni. *Journal of Chemical Theory and Computation*, **2007**, 3, 1349-67	6.4	177
75	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, 332-42	6.4	164
74	Electronic couplings for molecular charge transfer: benchmarking CDFT, FODFT, and FODFTB against high-level ab initio calculations. *Journal of Chemical Physics*, **2014**, 140, 104105	3.9	156
73	An approximate DFT method for QM/MM simulations of biological structures and processes. *Computational and Theoretical Chemistry*, **2003**, 632, 29-41		155
72	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, 565-81	3.5	146

71	Efficient calculation of charge-transfer matrix elements for hole transfer in DNA. *Journal of Physical Chemistry B*, **2008**, 112, 7937-47	3.4	135
70	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	3.9	132
69	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	2.3	128
68	Density functional tight binding: application to organic and biological molecules. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 49-61	7.9	127
67	Quantum mechanics simulation of protein dynamics on long timescale. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 484-9	4.2	127
66	Electronic couplings for molecular charge transfer: benchmarking CDFT, FODFT and FODFTB against high-level ab initio calculations. II. *Physical Chemistry Chemical Physics*, **2015**, 17, 14342-54	3.6	100
65	Density functional tight binding: values of semi-empirical methods in an ab initio era. *Physical Chemistry Chemical Physics*, **2014**, 16, 14368-77	3.6	98
64	Parametrization of DFTB3/3OB for magnesium and zinc for chemical and biological applications. *Journal of Physical Chemistry B*, **2015**, 119, 1062-82	3.4	90
63	From C2 Molecules to Self-Assembled Fullerenes in Quantum Chemical Molecular Dynamics. *Nano Letters*, **2003**, 3, 1657-1664	11.5	79
62	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	6.4	76
61	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, 11221-40	3.4	75
60	Simulating water with the self-consistent-charge density functional tight binding method: from molecular clusters to the liquid state. *Journal of Physical Chemistry A*, **2007**, 111, 5685-91	2.8	74
59	Combined density functional theory and Landauer approach for hole transfer in DNA along classical molecular dynamics trajectories. *Journal of Chemical Physics*, **2009**, 130, 215104	3.9	73
58	Application of the SCC-DFTB method to neutral and protonated water clusters and bulk water. *Journal of Physical Chemistry B*, **2011**, 115, 6790-805	3.4	71
57	A hybrid approach to simulation of electron transfer in complex molecular systems. *Journal of the Royal Society Interface*, **2013**, 10, 20130415	4.1	66
56	Automatized parametrization of SCC-DFTB repulsive potentials: application to hydrocarbons. *Journal of Physical Chemistry A*, **2009**, 113, 11866-81	2.8	63
55	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, 11462-7	3.4	60
54	Towards an understanding of channelrhodopsin function: simulations lead to novel insights of the channel mechanism. *Journal of Molecular Biology*, **2013**, 425, 1795-814	6.5	58

53	Size-Consistent Multipartitioning QM/MM: A Stable and Efficient Adaptive QM/MM Method. *Journal of Chemical Theory and Computation*, **2014**, 10, 4242-52	6.4	47
52	Effect of polarization on the opsin shift in rhodopsins. 2. Empirical polarization models for proteins. *Journal of Physical Chemistry B*, **2008**, 112, 11468-78	3.4	47
51	Formation of Fullerene Molecules from Carbon Nanotubes: A Quantum Chemical Molecular Dynamics Study. *Nano Letters*, **2003**, 3, 465-470	11.5	47
50	Time-Dependent Extension of the Long-Range Corrected Density Functional Based Tight-Binding Method. *Journal of Chemical Theory and Computation*, **2017**, 13, 1737-1747	6.4	46
49	Parametrization of the SCC-DFTB Method for Halogens. *Journal of Chemical Theory and Computation*, **2013**, 9, 2939-49	6.4	45
48	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, 11338-52	3.4	45
47	Multi-Scale Approach to Non-Adiabatic Charge Transport in High-Mobility Organic Semiconductors. *Journal of Chemical Theory and Computation*, **2015**, 11, 5068-82	6.4	44
46	Computational photochemistry of retinal proteins. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 511-8	4.2	44
45	Parametrization and Benchmark of Long-Range Corrected DFTB2 for Organic Molecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 115-125	6.4	41
44	Quantum Chemical Molecular Dynamics Model Study of Fullerene Formation from Open-Ended Carbon Nanotubes *Journal of Physical Chemistry A*, **2004**, 108, 3182-3194	2.8	39
43	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	6.4	39
42	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. *Journal of Chemical Physics*, **2015**, 143, 084123	3.9	38
41	Extended polarization in third-order SCC-DFTB from chemical-potential equalization. *Journal of Physical Chemistry A*, **2012**, 116, 9131-41	2.8	38
40	Reaction dynamics of the chimeric channelrhodopsin C1C2. *Scientific Reports*, **2017**, 7, 7217	4.9	37
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	6.4	36
38	Active site structure and absorption spectrum of channelrhodopsin-2 wild-type and C128T mutant. *Chemical Science*, **2016**, 7, 3879-3891	9.4	33
37	QM/QM approach to model energy disorder in amorphous organic semiconductors. *Journal of Chemical Theory and Computation*, **2015**, 11, 560-7	6.4	32
36	DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters. *Journal of Chemical Theory and Computation*, **2015**, 11, 4205-19	6.4	27

35	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	6.4	27
34	Color tuning in binding pocket models of the chlamydomonas-type channelrhodopsins. *Journal of Physical Chemistry B*, **2011**, 115, 15119-28	3.4	27
33	Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules. *Journal of Computational Chemistry*, **2017**, 38, 2171-2185	3.5	25
32	Simulation of Temperature-Dependent Charge Transport in Organic Semiconductors with Various Degrees of Disorder. *Journal of Chemical Theory and Computation*, **2016**, 12, 3087-96	6.4	25
31	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	3.6	22
30	Simulation of Singlet Exciton Diffusion in Bulk Organic Materials. *Journal of Chemical Theory and Computation*, **2016**, 12, 4209-21	6.4	21
29	Modeling charge transport in DNA using multi-scale methods. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 2277-2287	1.3	21
28	Charge and Exciton Transfer Simulations Using Machine-Learned Hamiltonians. *Journal of Chemical Theory and Computation*, **2020**, 16, 4061-4070	6.4	18
27	Improved electronic properties from third-order SCC-DFTB with cost efficient post-SCF extensions. *Journal of Physical Chemistry A*, **2012**, 116, 11927-37	2.8	15
26	Polaron Effects on Charge Transport through Molecular Wires: A Multiscale Approach. *Journal of Chemical Theory and Computation*, **2017**, 13, 286-296	6.4	14
25	DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. *Journal of Physical Chemistry Letters*, **2020**, 11, 8660-8667	6.4	14
24	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	6.4	13
23	Mechanism of a proton pump analyzed with computer simulations. *Theoretical Chemistry Accounts*, **2010**, 125, 353-363	1.9	13
22	Molecular Insights into Variable Electron Transfer in Amphibian Cryptochrome. *Biophysical Journal*, **2018**, 114, 2563-2572	2.9	12
21	On the mechanism of spontaneous thiol-disulfide exchange in proteins. *Physical Chemistry Chemical Physics*, **2018**, 20, 16222-16230	3.6	12
20	Mechanism by which untwisting of retinal leads to productive bacteriorhodopsin photocycle states. *Journal of Physical Chemistry B*, **2015**, 119, 2229-40	3.4	11
19	Computational study of synthetic agonist ligands of ionotropic glutamate receptors. *PLoS ONE*, **2013**, 8, e58774	3.7	11
18	Exploring the applicability of density functional tight binding to transition metal ions. Parameterization for nickel with the spin-polarized DFTB3 model. *Journal of Computational Chemistry*, **2019**, 40, 400-413	3.5	11

17	Multiscale QM/MM molecular dynamics simulations of the trimeric major light-harvesting complex II. *Physical Chemistry Chemical Physics*, **2021**, 23, 7407-7417	3.6	11
16	Relation between Dephasing Time and Energy Gap Fluctuations in Biomolecular Systems. *Journal of Physical Chemistry Letters*, **2016**, 7, 1102-8	6.4	10
15	Coupled-perturbed DFTB-QM/MM metadynamics: Application to proton-coupled electron transfer. *Journal of Chemical Physics*, **2018**, 149, 072328	3.9	8
14	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	3.9	6
13	Interplay of structural dynamics and electronic effects in an engineered assembly of pentacene in a metal-organic framework. *Chemical Science*, **2021**, 12, 4477-4483	9.4	6
12	Self-Consistent-Charge Density Functional Tight-Binding Method: An Efficient Approximation of Density Functional Theory **2011**, 287-307		5
11	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	6.4	5
10	"siRNA traffic lights": arabino-configured 2Ranchors for fluorescent dyes are key for dual color readout in cell imaging. *Organic and Biomolecular Chemistry*, **2018**, 16, 3726-3731	3.9	4
9	Molecular Dynamics Investigation of gluazo, a Photo-Switchable Ligand for the Glutamate Receptor GluK2. *PLoS ONE*, **2015**, 10, e0135399	3.7	4
8	Ligand photo-isomerization triggers conformational changes in iGluR2 ligand binding domain. *PLoS ONE*, **2014**, 9, e92716	3.7	4
7	Improvement of d-d interactions in density functional tight binding for transition metal ions with a ligand field model: assessment of a DFTB3+ model on nickel coordination compounds. *Physical Chemistry Chemical Physics*, **2020**, 22, 27084-27095	3.6	2
6	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	2.8	1
5	Hydrogen Storage in Single-Walled and Multi-Walled Carbon Nanotubes. *Materials Research Society Symposia Proceedings*, **1999**, 593, 187		1
4	Geometry dependence of excitonic couplings and the consequences for configuration-space sampling. *Journal of Computational Chemistry*, **2021**, 42, 1402-1418	3.5	1
3	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	6.4	1
2	Electrostatic interactions contribute to the control of intramolecular thiol-disulfide isomerization in a protein. *Physical Chemistry Chemical Physics*, **2021**, 23, 26366-26375	3.6	0
1	Efficient Surface Hopping Approach for Modeling Charge Transport in Organic Semiconductors.. *Journal of Chemical Theory and Computation*, **2022**, 18, 1264-1274	6.4	0