Thomas Frauenheim

List of Publications by Citations

574 papers	25,420 citations	78 h-index	139 g-index
602 ext. papers	27,733 ext. citations	4.6 avg, IF	7.06 L-index

#	Paper	IF	Citations
574	Construction of tight-binding-like potentials on the basis of density-functional theory: Application to carbon. *Physical Review B*, **1995**, 51, 12947-12957	3.3	1724
573	DFTB+, a sparse matrix-based implementation of the DFTB method. *Journal of Physical Chemistry A*, **2007**, 111, 5678-84	2.8	1327
572	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
571	Phosphorene as a Superior Gas Sensor: Selective Adsorption and Distinct I-V Response. *Journal of Physical Chemistry Letters*, **2014**, 5, 2675-81	6.4	723
570	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
569	Structure and electronic properties of MoS2 nanotubes. *Physical Review Letters*, **2000**, 85, 146-9	7.4	432
568	Oscillatory crossover from two-dimensional to three-dimensional topological insulators. *Physical Review B*, **2010**, 81,	3.3	389
567	Atomistic simulations of complex materials: ground-state and excited-state properties. *Journal of Physics Condensed Matter*, **2002**, 14, 3015-3047	1.8	384
566	Tight-binding molecular-dynamics simulation of impurities in ultrananocrystalline diamond grain boundaries. *Physical Review B*, **2001**, 65,	3.3	247
565	Two-dimensional Cu2Si monolayer with planar hexacoordinate copper and silicon bonding. *Journal of the American Chemical Society*, **2015**, 137, 2757-62	16.4	237
564	Accurate defect levels obtained from the HSE06 range-separated hybrid functional. *Physical Review B*, **2010**, 81,	3.3	224
563	Calculating absorption shifts for retinal proteins: computational challenges. *Journal of Physical Chemistry B*, **2005**, 109, 3606-15	3.4	221
562	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *Journal of Chemical Physics*, **2020**, 152, 124101	3.9	210
561	A hydrogen storage mechanism in single-walled carbon nanotubes. *Journal of the American Chemical Society*, **2001**, 123, 5059-63	16.4	210
560	Stability and electronic structure of GaN nanotubes from density-functional calculations. *Physical Review B*, **1999**, 60, 7788-7791	3.3	210
559	Tuning Magnetism and Electronic Phase Transitions by Strain and Electric Field in Zigzag MoS2 Nanoribbons. *Journal of Physical Chemistry Letters*, **2012**, 3, 2934-41	6.4	203
558	Silicon nanowire band gap modification. *Nano Letters*, **2007**, 7, 34-8	11.5	192

557	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. *Journal of Physical Chemistry C*, **2015**, 119, 6918-6922	3.8	184
556	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
555	The mechanism of diamond nucleation from energetic species. *Science*, **2002**, 297, 1531-3	33.3	179
554	Single-parent evolution algorithm and the optimization of Si clusters. *Physical Review Letters*, **2000**, 85, 546-9	7.4	179
553	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
552	Hydrogen adsorption and storage in carbon nanotubes. *Synthetic Metals*, **2000**, 113, 209-216	3.6	164
551	An Improved Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) Set of Parameters for Simulation of Bulk and Molecular Systems Involving Titanium. *Journal of Chemical Theory and Computation*, **2010**, 6, 266-78	6.4	155
550	An approximate DFT method for QM/MM simulations of biological structures and processes. *Computational and Theoretical Chemistry*, **2003**, 632, 29-41		155
549	Polaronic effects in TiO2 calculated by the HSE06 hybrid functional: Dopant passivation by carrier self-trapping. *Physical Review B*, **2011**, 83,	3.3	152
548	A global investigation of excited state surfaces within time-dependent density-functional response theory. *Journal of Chemical Physics*, **2004**, 120, 1674-92	3.9	149
547	Strain engineering of selective chemical adsorption on monolayer MoS2. *Nanoscale*, **2014**, 6, 5156-61	7.7	148
546	Quantitative theory of the oxygen vacancy and carrier self-trapping in bulk TiO2. *Physical Review B*, **2012**, 86,	3.3	147
545	Band Lineup and Charge Carrier Separation in Mixed Rutile-Anatase Systems. *Journal of Physical Chemistry C*, **2011**, 115, 3443-3446	3.8	147
544	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
543	Robust two-dimensional topological insulators in methyl-functionalized bismuth, antimony, and lead bilayer films. *Nano Letters*, **2015**, 15, 1083-9	11.5	145
542	Choosing the correct hybrid for defect calculations: A case study on intrinsic carrier trapping in □a2O3. *Physical Review B*, **2017**, 95,	3.3	144
541	Adsorption and desorption of an O2 molecule on carbon nanotubes. *Physical Review Letters*, **2000**, 85, 2757-60	7.4	144
540	Unraveling the Shape Transformation in Silicon Clusters. *Physical Review Letters*, **2004**, 93,	7.4	141

539	A critical evaluation of different QM/MM frontier treatments with SCC-DFTB as the QM method. *Journal of Physical Chemistry B*, **2005**, 109, 9082-95	3.4	138
538	Defects in SiO2 as the possible origin of near interface traps in the SiC/SiO2 system: A systematic theoretical study. *Physical Review B*, **2005**, 72,	3.3	134
537	Structure, stability, and vibrational properties of polymerized C60. *Physical Review B*, **1995**, 52, 14963-14970	3.3	134
536	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
535	Dark states of single nitrogen-vacancy centers in diamond unraveled by single shot NMR. *Physical Review Letters*, **2011**, 106, 157601	7.4	130
534	Decomposition of HMX at Extreme Conditions: A Molecular Dynamics Simulation. *Journal of Physical Chemistry A*, **2002**, 106, 9024-9029	2.8	129
533	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
532	Application of an approximate density-functional method to sulfur containing compounds. *Computational and Theoretical Chemistry*, **2001**, 541, 185-194		128
531	Quantum mechanics simulation of protein dynamics on long timescale. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 484-9	4.2	127
530	Nanoscale Multilayer Transition-Metal Dichalcogenide Heterostructures: Band Gap Modulation by Interfacial Strain and Spontaneous Polarization. *Journal of Physical Chemistry Letters*, **2013**, 4, 1730-6	6.4	126
529	Theoretical prediction of topological insulators in thallium-based III-V-VI 2 ternary chalcogenides. *Europhysics Letters*, **2010**, 90, 37002	1.6	126
528	Atomic structure and physical properties of amorphous carbon and its hydrogenated analogs. *Physical Review B*, **1993**, 48, 4823-4834	3.3	124
527	Theoretical study of the mechanism of dry oxidation of 4H-SiC. *Physical Review B*, **2005**, 71,	3.3	122
526	The mechanism of defect creation and passivation at the SiC/SiO2interface. *Journal Physics D: Applied Physics*, **2007**, 40, 6242-6253	3	120
525	Density functional based calculations for Fen (n?32). *Chemical Physics*, **2005**, 309, 23-31	2.3	120
524	Density-functional-based construction of transferable nonorthogonal tight-binding potentials for Si and SiH. *Physical Review B*, **1995**, 52, 11492-11501	3.3	119
523	Non-Markovian quantum processes: Complete framework and efficient characterization. *Physical Review A*, **2018**, 97,	2.6	114
522	Formation of NV centers in diamond: A theoretical study based on calculated transitions and migration of nitrogen and vacancy related defects. *Physical Review B*, **2014**, 89,	3.3	113

521	"Proton holes" in long-range proton transfer reactions in solution and enzymes: A theoretical analysis. *Journal of the American Chemical Society*, **2006**, 128, 16302-11	16.4	111
520	Stability, reconstruction, and electronic properties of diamond (100) and (111) surfaces. *Physical Review B*, **1993**, 48, 18189-18202	3.3	110
519	Resonant electron heating and molecular phonon cooling in single C60 junctions. *Physical Review Letters*, **2008**, 100, 136801	7.4	108
518	Electronic structures of GaN edge dislocations. *Physical Review B*, **2000**, 61, 16033-16039	3.3	107
517	Graphene-based topological insulator with an intrinsic bulk band gap above room temperature. *Nano Letters*, **2013**, 13, 6251-5	11.5	102
516	Toward an Accurate Density-Functional Tight-Binding Description of Zinc-Containing Compounds. *Journal of Chemical Theory and Computation*, **2009**, 5, 605-14	6.4	100
515	Incoherent Electron□Phonon Scattering in Octanethiols. *Nano Letters*, **2004**, 4, 2109-2114	11.5	100
514	Operational Markov Condition for Quantum Processes. *Physical Review Letters*, **2018**, 120, 040405	7.4	99
513	Dislocations in diamond: Core structures and energies. *Physical Review B*, **2002**, 65,	3.3	99
512	Structures and energetics of hydrogen-terminated silicon nanowire surfaces. *Journal of Chemical Physics*, **2005**, 123, 144703	3.9	98
511	pi bonding versus electronic-defect generation: An examination of band-gap properties in amorphous carbon. *Physical Review B*, **1994**, 50, 1489-1501	3.3	98
510	Understanding the inelastic electron-tunneling spectra of alkanedithiols on gold. *Journal of Chemical Physics*, **2006**, 124, 94704	3.9	96
509	Highly conductive boron nanotubes: transport properties, work functions, and structural stabilities. *ACS Nano*, **2011**, 5, 4997-5005	16.7	94
508	DFT studies on helix formation in N-acetyl-(L-alanyl)n-N?-methylamide for n=1□0. *Chemical Physics*, **2000**, 256, 15-27	2.3	94
507	Structure and shape variations in intermediate-size copper clusters. *Journal of Chemical Physics*, **2006**, 124, 024308	3.9	93
506	Proper surface termination for luminescent near-surface NV centers in diamond. *Nano Letters*, **2014**, 14, 4772-7	11.5	92
505	On the electronic structure of WS2 nanotubes. *Solid State Communications*, **2000**, 114, 245-248	1.6	92
504	Electronic structure of solid nitromethane: Effects of high pressure and molecular vacancies. *Journal of Chemical Physics*, **2002**, 117, 788-799	3.9	91

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502	Simulation of water cluster assembly on a graphite surface. *Journal of Physical Chemistry B*, **2005**, 109, 14183-8	3.4	89
501	New Family of Quantum Spin Hall Insulators in Two-dimensional Transition-Metal Halide with Large Nontrivial Band Gaps. *Nano Letters*, **2015**, 15, 7867-72	11.5	87
500	Structure and motion of basal dislocations in silicon carbide. *Physical Review B*, **2003**, 68,	3.3	83
499	Nonadiabatic Molecular Dynamics for Thousand Atom Systems: A Tight-Binding Approach toward PYXAID. *Journal of Chemical Theory and Computation*, **2016**, 12, 1436-48	6.4	82
498	Toward theoretical analysis of long-range proton transfer kinetics in biomolecular pumps. *Journal of Physical Chemistry A*, **2006**, 110, 548-63	2.8	82
497	11-cis-retinal protonated Schiff base: influence of the protein environment on the geometry of the rhodopsin chromophore. *Biochemistry*, **2002**, 41, 15259-66	3.2	78
496	Novel NbS2 metallic nanotubes. *Solid State Communications*, **2000**, 115, 635-638	1.6	78
495	A priori method for propensity rules for inelastic electron tunneling spectroscopy of single-molecule conduction. *Physical Review B*, **2007**, 75,	3.3	77
494	Molecular dynamics simulations of CFx (x=2,3) molecules at Si3N4 and SiO2 surfaces. *Surface Science*, **2006**, 600, 453-460	1.8	75
493	Molecular wires, solenoids, and capacitors by sidewall functionalization of carbon nanotubes. *Applied Physics Letters*, **2000**, 77, 1313-1315	3.4	75
492	Approximate density-functional calculations of spin densities in large molecular systems and complex solids. *Physical Chemistry Chemical Physics*, **2001**, 3, 5109-5114	3.6	75
491	Robust 2D topological insulators in van der Waals heterostructures. *ACS Nano*, **2014**, 8, 10448-54	16.7	74
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489	Revealing unusual chemical bonding in planar hyper-coordinate Ni2Ge and quasi-planar Ni2Si two-dimensional crystals. *Physical Chemistry Chemical Physics*, **2015**, 17, 26043-8	3.6	73
488	Response of C60 and Cn to ultrashort laser pulses. *Physical Review B*, **2001**, 64,	3.3	72
487	Geometric and Electronic Structures of Carbon Nanotubes Adsorbed with Flavin Adenine Dinucleotide: A Theoretical Study. *Journal of Physical Chemistry C*, **2007**, 111, 4069-4073	3.8	69
486	Structural evolution of anionic silicon clusters SiN (20 . *Journal of Physical Chemistry A*, **2006**, 110, 908-12	2.8	69

485	Structural and electronic properties of ZnO nanotubes from density functional calculations. *Nanotechnology*, **2007**, 18, 485713	3.4	68
484	Density-functional-based predictions of Raman and IR spectra for small Si clusters. *Physical Review B*, **1997**, 55, 2549-2555	3.3	67
483	Stability, chemical bonding, and vibrational properties of amorphous carbon at different mass densities. *Physical Review B*, **1995**, 52, 11837-11844	3.3	66
482	High-Throughput Screening of Synergistic Transition Metal Dual-Atom Catalysts for Efficient Nitrogen Fixation. *Nano Letters*, **2021**, 21, 1871-1878	11.5	66
481	Post-anti-van't Hoff-Le Bel motif in atomically thin germanium-copper alloy film. *Physical Chemistry Chemical Physics*, **2015**, 17, 17545-51	3.6	65
480	Density-functional based tight-binding study of small gold clusters. *New Journal of Physics*, **2006**, 8, 9-9	2.9	65
479	Rare-earth defect pairs in GaN: LDA+U calculations. *Physical Review B*, **2009**, 80,	3.3	64
478	Hybrid SCC-DFTB/molecular mechanical studies of H-bonded systems and of N-acetyl-(L-Ala)n N?-methylamide helices in water solution. *International Journal of Quantum Chemistry*, **2000**, 78, 459-479	2.1	64
477	Origin of photoluminescence in □a2O3. *Physical Review B*, **2018**, 97,	3.3	63
476	Theoretical tools for transport in molecular nanostructures. *Physica B: Condensed Matter*, **2002**, 314, 86-90	2.8	63
475	Effect of oxygen on the growth of (101 0) GaN surfaces: The formation of nanopipes. *Applied Physics Letters*, **1998**, 73, 3530-3532	3.4	61
474	Intense intrashell luminescence of Eu-doped single ZnO nanowires at room temperature by implantation created Eu-Oi complexes. *Nano Letters*, **2014**, 14, 4523-8	11.5	60
473	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
472	Shape, polarizability, and metallicity in silicon clusters. *Physical Review A*, **2005**, 71,	2.6	60
471	Unusual size dependence of the optical emission gap in small hydrogenated silicon nanoparticles. *Applied Physics Letters*, **2007**, 90, 123116	3.4	59
470	Charge corrections for supercell calculations of defects in semiconductors. *Physica B: Condensed Matter*, **2003**, 340-342, 190-194	2.8	59
469	SCC-DFTB parameters for simulating hybrid gold-thiolates compounds. *Journal of Computational Chemistry*, **2015**, 36, 2075-87	3.5	58
468	Theoretical study of the chemical gap tuning in silicon nanowires. *Physical Review B*, **2007**, 76,	3.3	58

467	Theoretical investigation of carbon defects and diffusion in α-quartz. *Physical Review B*, **2001**, 64,	3.3	58
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465	Fingerprints of order and disorder in the electronic and optical properties of crystalline and amorphous TiO2. *Physical Review B*, **2012**, 86,	3.3	56
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461	Predicting Two-Dimensional CB/CN van der Waals p-n Heterojunction with Strong Interlayer Electron Coupling and Enhanced Photocurrent. *Journal of Physical Chemistry Letters*, **2018**, 9, 858-862	6.4	55
460	Structural properties of amorphous hydrogenated carbon. IV. A molecular-dynamics investigation and comparison to experiments. *Physical Review B*, **1994**, 50, 6709-6716	3.3	55
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456	Optimal surface functionalization of silicon quantum dots. *Journal of Chemical Physics*, **2008**, 128, 244714	3.9	53
455	Extensions of the Time-Dependent Density Functional Based Tight-Binding Approach. *Journal of Chemical Theory and Computation*, **2013**, 9, 4901-14	6.4	51
454	Treatment of collinear and noncollinear electron spin within an approximate density functional based method. *Journal of Physical Chemistry A*, **2007**, 111, 5622-9	2.8	51
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448	Observation of "Stick" and "Handle" intermediates along the fullerene road. *Physical Review Letters* , **2000**, 84, 2421-4	7.4	49
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446	Water splitting and the band edge positions of TiO2. *Electrochimica Acta*, **2016**, 199, 27-34	6.7	48
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443	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
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440	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
439	Hydrogen and oxygen adsorption on ZnO nanowires: A first-principles study. *Physical Review B*, **2009**, 79,	3.3	46
438	Quasiparticle energies for large molecules: A tight-binding-based Green□-function approach. *Physical Review A*, **2005**, 71,	2.6	46
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435	Parametrization of the SCC-DFTB Method for Halogens. *Journal of Chemical Theory and Computation*, **2013**, 9, 2939-49	6.4	45
434	Theoretical Insights into CO2 Activation and Reduction on the Ag(111) Monolayer Supported on a ZnO(0001) Substrate. *Journal of Physical Chemistry C*, **2013**, 117, 1804-1808	3.8	45
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425	Electronic structure of dense amorphous carbon. *Physical Review B*, **1994**, 49, 11448-11451	3.3	43
424	Resolving the Controversy about the Band Alignment between Rutile and Anatase: The Role of OH/H+ Adsorption. *Journal of Physical Chemistry C*, **2015**, 119, 21952-21958	3.8	42
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418	Calculation of carrier-concentration-dependent effective mass in Nb-doped anatase crystals of TiO2. *Physical Review B*, **2011**, 83,	3.3	41
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406	Analysis of band-gap formation in squashed armchair carbon nanotubes. *Physical Review B*, **2005**, 71,	3.3	37
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404	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. *Chemical Science*, **2014**, 5, 3493-3500	9.4	36
403	An SCC-DFTB/MD Study of the Adsorption of Zwitterionic Glycine on a Geminal Hydroxylated Silica Surface in an Explicit Water Environment. *Journal of Physical Chemistry C*, **2011**, 115, 9615-9621	3.8	36
402	Analytical excited state forces for the time-dependent density-functional tight-binding method. *Journal of Computational Chemistry*, **2007**, 28, 2589-601	3.5	36
401	An SCC-DFTB Repulsive Potential for Various ZnO Polymorphs and the ZnO-Water System. *Journal of Physical Chemistry C*, **2013**, 117, 17004-17015	3.8	35
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