Thomas Frauenheim

List of Publications by Year
in descending order

589	30,043	4641 85	7496 151
papers	citations	h-index	g-index

602	602	602	22883
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Construction of tight-binding-like potentials on the basis of density-functional theory: Application to carbon. Physical Review B, 1995, 51, 12947-12957.	1.1	1,950
2	DFTB+, a Sparse Matrix-Based Implementation of the DFTB Methodâ€. Journal of Physical Chemistry A, 2007, 111, 5678-5684.	1.1	1,523
3	Hydrogen bonding and stacking interactions of nucleic acid base pairs: A density-functional-theory based treatment. Journal of Chemical Physics, 2001, 114, 5149-5155.	1.2	978
4	Phosphorene as a Superior Gas Sensor: Selective Adsorption and Distinct Iâ€“V Response. Journal of Physical Chemistry Letters, 2014, 5, 2675-2681.	2.1	877
5	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
6	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.	1.2	568
7	Structure and Electronic Properties ofMoS2Nanotubes. Physical Review Letters, 2000, 85, 146-149.	2.9	497
8	Oscillatory crossover from two-dimensional to three-dimensional topological insulators. Physical Review B, 2010, 81, .	1.1	459
9	Atomistic simulations of complex materials: ground-state and excited-state properties. Journal of Physics Condensed Matter, 2002, 14, 3015-3047.	0.7	423
10	Two-Dimensional Cu₂Si Monolayer with Planar Hexacoordinate Copper and Silicon Bonding. Journal of the American Chemical Society, 2015, 137, 2757-2762.	6.6	335
11	Accurate defect levels obtained from the HSE06 range-separated hybrid functional. Physical Review B, 2010, 81, .	1.1	297
12	Tight-binding molecular-dynamics simulation of impurities in ultrananocrystalline diamond grain boundaries. Physical Review B, 2001, 65, .	1.1	267
13	Calculating Absorption Shifts for Retinal Proteins:Â Computational Challenges. Journal of Physical Chemistry B, 2005, 109, 3606-3615.	1.2	237
14	Stability and electronic structure of GaN nanotubes from density-functional calculations. Physical Review B, 1999, 60, 7788-7791.	1.1	231
15	Tuning Magnetism and Electronic Phase Transitions by Strain and Electric Field in Zigzag MoS₂ Nanoribbons. Journal of Physical Chemistry Letters, 2012, 3, 2934-2941.	2.1	229
16	A Hydrogen Storage Mechanism in Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2001, 123, 5059-5063.	6.6	227
17	High-Throughput Screening of Synergistic Transition Metal Dual-Atom Catalysts for Efficient Nitrogen Fixation. Nano Letters, 2021, 21, 1871-1878.	4.5	223
18	Silicon Nanowire Band Gap Modification. Nano Letters, 2007, 7, 34-38.	4.5	215

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19	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. Journal of Physical Chemistry C, 2015, 119, 6918-6922.	1.5	210
20	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.	2.3	208
21	The Mechanism of Diamond Nucleation from Energetic Species. Science, 2002, 297, 1531-1533.	6.0	202
22	Non-Markovian quantum processes: Complete framework and efficient characterization. Physical Review A, 2018, 97, .	1.0	202
23	Hydrogen adsorption and storage in carbon nanotubes. Synthetic Metals, 2000, 113, 209-216.	2.1	196
24	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.	6.6	196
25	Single-Parent Evolution Algorithm and the Optimization of Si Clusters. Physical Review Letters, 2000, 85, 546-549.	2.9	189
26	Choosing the correct hybrid for defect calculations: A case study on intrinsic carrier trapping in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">G</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical	1.1	184
27	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, 266-278.	2.3	177
28	Strain engineering of selective chemical adsorption on monolayer MoS₂. Nanoscale, 2014, 6, 5156-5161.	2.8	177
29	Polaronic effects in TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>calculated by the HSE06 hybrid functional: Dopant passivation by carrier self-trapping. Physical Review B, 2011, 83, .	1.1	176
30	An approximate DFT method for QM/MM simulations of biological structures and processes. Computational and Theoretical Chemistry, 2003, 632, 29-41.	1.5	172
31	Quantitative theory of the oxygen vacancy and carrier self-trapping in bulk TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	169
32	Robust Two-Dimensional Topological Insulators in Methyl-Functionalized Bismuth, Antimony, and Lead Bilayer Films. Nano Letters, 2015, 15, 1083-1089.	4.5	166
33	Application of an approximate density-functional method to sulfur containing compounds. Computational and Theoretical Chemistry, 2001, 541, 185-194.	1.5	165
34	Band Lineup and Charge Carrier Separation in Mixed Rutile-Anatase Systems. Journal of Physical Chemistry C, 2011, 115, 3443-3446.	1.5	162
35	Operational Markov Condition for Quantum Processes. Physical Review Letters, 2018, 120, 040405.	2.9	157
36	A Critical Evaluation of Different QM/MM Frontier Treatments with SCC-DFTB as the QM Method. Journal of Physical Chemistry B, 2005, 109, 9082-9095.	1.2	156

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37	Dark States of Single Nitrogen-Vacancy Centers in Diamond Unraveled by Single Shot NMR. Physical Review Letters, 2011, 106, 157601.	2.9	156
38	A global investigation of excited state surfaces within time-dependent density-functional response theory. Journal of Chemical Physics, 2004, 120, 1674-1692.	1.2	151
39	Defects inSiO2as the possible origin of near interface traps in theSiCâ•SiO2system: A systematic theoretical study. Physical Review B, 2005, 72, .	1.1	151
40	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.	1.5	150
41	Unraveling the Shape Transformation in Silicon Clusters. Physical Review Letters, 2004, 93, .	2.9	150
42	Adsorption and Desorption of anO2Molecule on Carbon Nanotubes. Physical Review Letters, 2000, 85, 2757-2760.	2.9	149
43	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, .	1.1	149
44	Density functional based calculations for Fen (nâ©½32). Chemical Physics, 2005, 309, 23-31.	0.9	146
45	Decomposition of HMX at Extreme Conditions:Â A Molecular Dynamics Simulation. Journal of Physical Chemistry A, 2002, 106, 9024-9029.	1.1	145
46	The mechanism of defect creation and passivation at the SiC/SiO₂interface. Journal Physics D: Applied Physics, 2007, 40, 6242-6253.	1.3	143
47	Nanoscale Multilayer Transition-Metal Dichalcogenide Heterostructures: Band Gap Modulation by Interfacial Strain and Spontaneous Polarization. Journal of Physical Chemistry Letters, 2013, 4, 1730-1736.	2.1	142
48	Quantum mechanics simulation of protein dynamics on long timescale. Proteins: Structure, Function and Bioinformatics, 2001, 44, 484-489.	1.5	140
49	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.	1.2	140
50	Theoretical prediction of topological insulators in thallium-based III-V-VI ₂ ternary chalcogenides. Europhysics Letters, 2010, 90, 37002.	0.7	140
51	Structure, stability, and vibrational properties of polymerizedC60. Physical Review B, 1995, 52, 14963-14970.	1.1	139
52	Density-functional-based construction of transferable nonorthogonal tight-binding potentials for Si and SiH. Physical Review B, 1995, 52, 11492-11501.	1.1	133
53	Theoretical study of the mechanism of dry oxidation of4H-SiC. Physical Review B, 2005, 71, .	1.1	133
54	Atomic structure and physical properties of amorphous carbon and its hydrogenated analogs. Physical Review B, 1993, 48, 4823-4834.	1.1	132

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55	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.	0.9	132
56	â€œProton Holesâ€•in Long-Range Proton Transfer Reactions in Solution and Enzymes:Â A Theoretical Analysis. Journal of the American Chemical Society, 2006, 128, 16302-16311.	6.6	125
57	Proper Surface Termination for Luminescent Near-Surface NV Centers in Diamond. Nano Letters, 2014, 14, 4772-4777.	4.5	125
58	On the electronic structure of WS2 nanotubes. Solid State Communications, 2000, 114, 245-248.	0.9	120
59	Resonant Electron Heating and Molecular Phonon Cooling in Single<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>Junctions. Physical Review Letters, 2008, 100, 136801.	2.9	120
60	Stability, reconstruction, and electronic properties of diamond (100) and (111) surfaces. Physical Review B, 1993, 48, 18189-18202.	1.1	118
61	Electronic structures of GaN edge dislocations. Physical Review B, 2000, 61, 16033-16039.	1.1	117
62	Graphene-Based Topological Insulator with an Intrinsic Bulk Band Gap above Room Temperature. Nano Letters, 2013, 13, 6251-6255.	4.5	116
63	Dislocations in diamond: Core structures and energies. Physical Review B, 2002, 65, .	1.1	114
64	Toward an Accurate Density-Functional Tight-Binding Description of Zinc-Containing Compounds. Journal of Chemical Theory and Computation, 2009, 5, 605-614.	2.3	113
65	Structures and energetics of hydrogen-terminated silicon nanowire surfaces. Journal of Chemical Physics, 2005, 123, 144703.	1.2	109
66	Incoherent Electronâ^'Phonon Scattering in Octanethiols. Nano Letters, 2004, 4, 2109-2114.	4.5	106
67	Highly Conductive Boron Nanotubes: Transport Properties, Work Functions, and Structural Stabilities. ACS Nano, 2011, 5, 4997-5005.	7.3	106
68	New Family of Quantum Spin Hall Insulators in Two-dimensional Transition-Metal Halide with Large Nontrivial Band Gaps. Nano Letters, 2015, 15, 7867-7872.	4.5	104
69	Origin of photoluminescence in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">G</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 97, .	1.1	104
70	Ï€ bonding versus electronic-defect generation: An examination of band-gap properties in amorphous carbon. Physical Review B, 1994, 50, 1489-1501.	1.1	103
71	Understanding the inelastic electron-tunneling spectra of alkanedithiols on gold. Journal of Chemical Physics, 2006, 124, 094704.	1.2	103
72	Structure and shape variations in intermediate-size copper clusters. Journal of Chemical Physics, 2006, 124, 024308.	1.2	100

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73	Controllable Magnetic Doping of the Surface State of a Topological Insulator. Physical Review Letters, 2013, 110, 126804.	2.9	98
74	DFT studies on helix formation in N-acetyl-(L-alanyl)n-Nâ€²-methylamide for n=1â€“20. Chemical Physics, 2000, 256, 15-27.	0.9	96
75	Novel NbS2 metallic nanotubes. Solid State Communications, 2000, 115, 635-638.	0.9	95
76	Electronic structure of solid nitromethane: Effects of high pressure and molecular vacancies. Journal of Chemical Physics, 2002, 117, 788-799.	1.2	95
77	Simulation of Water Cluster Assembly on a Graphite Surface. Journal of Physical Chemistry B, 2005, 109, 14183-14188.	1.2	95
78	Toward Theoretical Analyis of Long-Range Proton Transfer Kinetics in Biomolecular Pumpsâ€. Journal of Physical Chemistry A, 2006, 110, 548-563.	1.1	95
79	Revealing unusual chemical bonding in planar hyper-coordinate Ni₂Ge and quasi-planar Ni₂Si two-dimensional crystals. Physical Chemistry Chemical Physics, 2015, 17, 26043-26048.	1.3	95
80	Ni/Mo Bimetallicâ€Oxideâ€Derived Heterointerfaceâ€Rich Sulfide Nanosheets with Coâ€Doping for Efficient Alkaline Hydrogen Evolution by Boosting Volmer Reaction. Small, 2021, 17, e2006730.	5.2	95
81	Performance of the AM1, PM3, and SCC-DFTB methods in the study of conjugated Schiff base molecules. Chemical Physics, 2002, 277, 91-103.	0.9	93
82	Molecular dynamics simulations of CFx (x=2,3) molecules at Si3N4 and SiO2 surfaces. Surface Science, 2006, 600, 453-460.	0.8	93
83	Nonadiabatic Molecular Dynamics for Thousand Atom Systems: A Tight-Binding Approach toward PYXAID. Journal of Chemical Theory and Computation, 2016, 12, 1436-1448.	2.3	93
84	Structure and motion of basal dislocations in silicon carbide. Physical Review B, 2003, 68, .	1.1	92
85	Robust 2D Topological Insulators in van der Waals Heterostructures. ACS Nano, 2014, 8, 10448-10454.	7.3	88
86	Molecular wires, solenoids, and capacitors by sidewall functionalization of carbon nanotubes. Applied Physics Letters, 2000, 77, 1313-1315.	1.5	86
87	Approximate density-functional calculations of spin densities in large molecular systems and complex solids. Physical Chemistry Chemical Physics, 2001, 3, 5109-5114.	1.3	82
88	11-cis-Retinal Protonated Schiff Base:Â Influence of the Protein Environment on the Geometry of the Rhodopsin Chromophoreâ€. Biochemistry, 2002, 41, 15259-15266.	1.2	82
89	SCCâ€DFTB parameters for simulating hybrid goldâ€thiolates compounds. Journal of Computational Chemistry, 2015, 36, 2075-2087.	1.5	82
90	Post-anti-van't Hoff-Le Bel motif in atomically thin germaniumâ€“copper alloy film. Physical Chemistry Chemical Physics, 2015, 17, 17545-17551.	1.3	81

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91	A priorimethod for propensity rules for inelastic electron tunneling spectroscopy of single-molecule conduction. Physical Review B, 2007, 75, .	1.1	80
92	Theoretical investigation of carbon defects and diffusion in Î±-quartz. Physical Review B, 2001, 64, .	1.1	75
93	Response ofC60andCnto ultrashort laser pulses. Physical Review B, 2001, 64, .	1.1	75
94	Theoretical tools for transport in molecular nanostructures. Physica B: Condensed Matter, 2002, 314, 86-90.	1.3	75
95	Structural Evolution of Anionic Silicon Clusters SiN(20 â‰Nâ‰ 45). Journal of Physical Chemistry A, 2006, 110, 908-912.	1.1	75
96	Geometric and Electronic Structures of Carbon Nanotubes Adsorbed with Flavin Adenine Dinucleotide:â€‰ A Theoretical Study. Journal of Physical Chemistry C, 2007, 111, 4069-4073.	1.5	74
97	Predicting Two-Dimensional C₃B/C₃N van der Waals pâ€“n Heterojunction with Strong Interlayer Electron Coupling and Enhanced Photocurrent. Journal of Physical Chemistry Letters, 2018, 9, 858-862.	2.1	74
98	Toward Rational Design of Catalysts Supported on a Topological Insulator Substrate. ACS Catalysis, 2015, 5, 7063-7067.	5.5	73
99	Density-functional based tight-binding study of small gold clusters. New Journal of Physics, 2006, 8, 9-9.	1.2	72
100	Structural and electronic properties of ZnO nanotubes from density functional calculations. Nanotechnology, 2007, 18, 485713.	1.3	72
101	Density-functional-based predictions of Raman and IR spectra for small Si clusters. Physical Review B, 1997, 55, 2549-2555.	1.1	71
102	Stability, chemical bonding, and vibrational properties of amorphous carbon at different mass densities. Physical Review B, 1995, 52, 11837-11844.	1.1	70
103	Rare-earth defect pairs in GaN:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>LDA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> Physical Review B, 2009, 80, .	1.1	70
104	SiC₇siligraphene: a novel donor material with extraordinary sunlight absorption. Nanoscale, 2016, 8, 6994-6999.	2.8	70
105	Hybrid SCC-DFTB/molecular mechanical studies of H-bonded systems and ofN-acetyl-(L-Ala)nN?-methylamide helices in water solution. International Journal of Quantum Chemistry, 2000, 78, 459-479.	1.0	68
106	Glitter in a 2D monolayer. Physical Chemistry Chemical Physics, 2015, 17, 26036-26042.	1.3	68
107	Quantum spin Hall states in graphene interacting with WS2 or WSe2. Applied Physics Letters, 2014, 105, .	1.5	67
108	Time-Dependent Extension of the Long-Range Corrected Density Functional Based Tight-Binding Method. Journal of Chemical Theory and Computation, 2017, 13, 1737-1747.	2.3	67

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109	Effect of oxygen on the growth of (101Ì„0) GaN surfaces: The formation of nanopipes. Applied Physics Letters, 1998, 73, 3530-3532.	1.5	66
110	Stoichiometric and non-stoichiometric (101Ì„0) and (112Ì„0) surfaces in 2Hâ€“SiC: a theoretical study. Solid State Communications, 1999, 111, 459-464.	0.9	66
111	Theoretical study of the chemical gap tuning in silicon nanowires. Physical Review B, 2007, 76, .	1.1	65
112	Fingerprints of order and disorder in the electronic and optical properties of crystalline and amorphous TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	65
113	Water splitting and the band edge positions of TiO2. Electrochimica Acta, 2016, 199, 27-34.	2.6	64
114	Intense Intrashell Luminescence of Eu-Doped Single ZnO Nanowires at Room Temperature by Implantation Created Euâ€“O_i Complexes. Nano Letters, 2014, 14, 4523-4528.	4.5	63
115	Shape transition of medium-sized neutral silicon clusters. Physica Status Solidi (B): Basic Research, 2003, 240, 537-548.	0.7	62
116	Tubular structures of GaS. Physical Review B, 2004, 69, .	1.1	62
117	Shape, polarizability, and metallicity in silicon clusters. Physical Review A, 2005, 71, .	1.0	62
118	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.	1.2	62
119	Stability of large vacancy clusters in silicon. Physical Review B, 2002, 65, .	1.1	61
120	Unusual size dependence of the optical emission gap in small hydrogenated silicon nanoparticles. Applied Physics Letters, 2007, 90, 123116.	1.5	61
121	Charge corrections for supercell calculations of defects in semiconductors. Physica B: Condensed Matter, 2003, 340-342, 190-194.	1.3	60
122	Versatile Single-Layer Sodium Phosphidostannate(II): Strain-Tunable Electronic Structure, Excellent Mechanical Flexibility, and an Ideal Gap for Photovoltaics. Journal of Physical Chemistry Letters, 2015, 6, 2682-2687.	2.1	60
123	Structural properties of amorphous hydrogenated carbon. IV. A molecular-dynamics investigation and comparison to experiments. Physical Review B, 1994, 50, 6709-6716.	1.1	59
124	First-principles calculations of reconstructed [0001] ZnO nanowires. Physical Review B, 2007, 76, .	1.1	58
125	Dislocations in diamond: Dissociation into partials and their glide motion. Physical Review B, 2003, 68, .	1.1	57
126	Optimal surface functionalization of silicon quantum dots. Journal of Chemical Physics, 2008, 128, 244714.	1.2	57

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127	Extensions of the Time-Dependent Density Functional Based Tight-Binding Approach. Journal of Chemical Theory and Computation, 2013, 9, 4901-4914.	2.3	57
128	Oxygen deficiency in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: Similarities and differences between the Ti self-interstitial and the O vacancy in bulk rutile and anatase. Physical Review B, 2015, 92, .	1.1	57
129	Doped graphenes as anodes with large capacity for lithium-ion batteries. Journal of Materials Chemistry A, 2016, 4, 13407-13413.	5.2	57
130	Dislocation Related Photoluminescence in Silicon. Physical Review Letters, 2001, 87, .	2.9	55
131	Treatment of Collinear and Noncollinear Electron Spin within an Approximate Density Functional Based Methodâ€. Journal of Physical Chemistry A, 2007, 111, 5622-5629.	1.1	55
132	Structure and elastic properties of amorphous silicon carbon nitride films. Physical Review B, 2001, 64, .	1.1	54
133	Parametrization of the SCC-DFTB Method for Halogens. Journal of Chemical Theory and Computation, 2013, 9, 2939-2949.	2.3	54
134	Coexistence of Three Ferroic Orders in the Multiferroic Compound [(CH₃)₄N][Mn(N₃)₃] with Perovskiteâ€Like Structure. Chemistry - A European Journal, 2016, 22, 7863-7870.	1.7	54
135	Influence of dislocations on electron energy-loss spectra in gallium nitride. Physical Review B, 2002, 65, .	1.1	53
136	New proton conducting hybrid membranes for HT-PEMFC systems based on polysiloxanes and SO3H-functionalized mesoporous Si-MCM-41 particles. Journal of Membrane Science, 2008, 316, 164-175.	4.1	53
137	Observation of â€œStickâ€•and â€œHandleâ€•Intermediates along the Fullerene Road. Physical Review Letters, 2000, 84, 2421-2424.	2.9	52
138	Self-Interaction and Strong Correlation in DFTBâ€. Journal of Physical Chemistry A, 2007, 111, 5671-5677.	1.1	52
139	The new dimension of silver. Physical Chemistry Chemical Physics, 2015, 17, 19695-19699.	1.3	52
140	Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies. Journal of Physical Chemistry B, 2016, 120, 7297-7306.	1.2	52
141	Dynamic properties and structure formation of boron and carbon nitrides. Diamond and Related Materials, 1996, 5, 1031-1041.	1.8	51
142	Quasiparticle energies for large molecules: A tight-binding-based Greenâ€™s-function approach. Physical Review A, 2005, 71, .	1.0	51
143	Hydrogen and oxygen adsorption on ZnO nanowires: A first-principles study. Physical Review B, 2009, 79, .	1.1	51
144	Novel Excitonic Solar Cells in Phosphoreneâ€“TiO₂ Heterostructures with Extraordinary Charge Separation Efficiency. Journal of Physical Chemistry Letters, 2016, 7, 1880-1887.	2.1	51

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145	Plasmon-induced hot-carrier generation differences in gold and silver nanoclusters. Nanoscale, 2019, 11, 8604-8615.	2.8	51
146	Importance of electronic self-consistency in the TDDFT based treatment of nonadiabatic molecular dynamics. European Physical Journal D, 2005, 35, 467-477.	0.6	50
147	Computational photochemistry of retinal proteins. Journal of Computer-Aided Molecular Design, 2006, 20, 511-518.	1.3	50
148	Covalent functionalization of ZnO surfaces: A density functional tight binding study. Applied Physics Letters, 2009, 94, 193109.	1.5	50
149	Theoretical Insights into CO₂ Activation and Reduction on the Ag(111) Monolayer Supported on a ZnO(000<u>1</u>) Substrate. Journal of Physical Chemistry C, 2013, 117, 1804-1808.	1.5	50
150	Effect of Polarization on the Opsin Shift in Rhodopsins. 2. Empirical Polarization Models for Proteins. Journal of Physical Chemistry B, 2008, 112, 11468-11478.	1.2	49
151	Theoretical prediction of topological insulator in ternary rare earth chalcogenides. Physical Review B, 2010, 82, .	1.1	49
152	Absorption and luminescence spectra of electroluminescent liquid crystals with triphenylene, pyrene and perylene units. Liquid Crystals, 2001, 28, 1105-1113.	0.9	48
153	Observation of R30Â° diamond (111) on vapour-grown polycrystalline films. Surface Science, 1993, 295, 340-346.	0.8	47
154	Dislocations in diamond: Electron energy-loss spectroscopy. Physical Review B, 2002, 65, .	1.1	47
155	Time-dependent versus static quantum transport simulations beyond linear response. Physical Review B, 2011, 83, .	1.1	47
156	Electronic structure of dense amorphous carbon. Physical Review B, 1994, 49, 11448-11451.	1.1	46
157	Excitations, optical absorption spectra, and optical excitonic gaps of heterofullerenes. I. C60, C59N+, and C48N12:â€,Theory and experiment. Journal of Chemical Physics, 2004, 120, 5133-5147.	1.2	46
158	Polarons and oxygen vacancies at the surface of anatase TiO₂. Physica Status Solidi - Rapid Research Letters, 2014, 8, 583-586.	1.2	46
159	Self-Consistent-Charge Density-Functional Tight-Binding Parameters for Cdâ€“X (X = S, Se, Te) Compounds and Their Interaction with H, O, C, and N. Journal of Chemical Theory and Computation, 2011, 7, 2262-2276.	2.3	45
160	Calculation of carrier-concentration-dependent effective mass in Nb-doped anatase crystals of TiO2. Physical Review B, 2011, 83, .	1.1	45
161	Energy partition inC60-diamond-(111)-surface collisions: A molecular-dynamics simulation. Physical Review B, 1994, 49, 11409-11414.	1.1	44
162	Evidence for Fe²⁺ in Wurtzite Coordination: Iron Doping Stabilizes ZnO Nanoparticles. Small, 2011, 7, 2879-2886.	5.2	44

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163	Self-Consistent Potential Correction for Charged Periodic Systems. Physical Review Letters, 2021, 126, 076401.	2.9	44
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