Stephan Irle

List of Publications by Year
in descending order

277 papers	14,688 citations	19608 61 h-index	24915 109 g-index
305 all docs	305 docs citations	305 times ranked	14404 citing authors

#	Article	IF	Citations
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
2	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
3	Conjugated organic framework with three-dimensionally ordered stable structure and delocalized Ï€ clouds. Nature Communications, 2013, 4, 2736.	5.8	528
4	In Operando X-ray Absorption Fine Structure Studies of Polyoxometalate Molecular Cluster Batteries: Polyoxometalates as Electron Sponges. Journal of the American Chemical Society, 2012, 134, 4918-4924.	6.6	385
5	Highâ€Rate Chargeâ€Carrier Transport in Porphyrin Covalent Organic Frameworks: Switching from Hole to Electron to Ambipolar Conduction. Angewandte Chemie - International Edition, 2012, 51, 2618-2622.	7.2	344
6	An n-Channel Two-Dimensional Covalent Organic Framework. Journal of the American Chemical Society, 2011, 133, 14510-14513.	6.6	330
7	Locking Covalent Organic Frameworks with Hydrogen Bonds: General and Remarkable Effects on Crystalline Structure, Physical Properties, and Photochemical Activity. Journal of the American Chemical Society, 2015, 137, 3241-3247.	6.6	320
8	Catalytic covalent organic frameworks via pore surface engineering. Chemical Communications, 2014, 50, 1292-1294.	2.2	292
9	Rational design of crystalline supermicroporous covalent organic frameworks with triangular topologies. Nature Communications, 2015, 6, 7786.	5.8	274
10	Charge Dynamics in A Donorâ€“Acceptor Covalent Organic Framework with Periodically Ordered Bicontinuous Heterojunctions. Angewandte Chemie - International Edition, 2013, 52, 2017-2021.	7.2	263
11	An Ambipolar Conducting Covalent Organic Framework with Selfâ€Sorted and Periodic Electron Donorâ€Acceptor Ordering. Advanced Materials, 2012, 24, 3026-3031.	11.1	258
12	Control of Crystallinity and Porosity of Covalent Organic Frameworks by Managing Interlayer Interactions Based on Self-Complementary Ï€-Electronic Force. Journal of the American Chemical Society, 2013, 135, 546-549.	6.6	257
13	Combined experimental and theoretical studies on the photophysical properties of cycloparaphenylenes. Organic and Biomolecular Chemistry, 2012, 10, 5979.	1.5	248
14	The C60Formation Puzzle â€œSolvedâ€Â QM/MD Simulations Reveal the Shrinking Hot Giant Road of the Dynamic Fullerene Self-Assembly Mechanism. Journal of Physical Chemistry B, 2006, 110, 14531-14545.	1.2	232
15	Creation of Superheterojunction Polymers via Direct Polycondensation: Segregated and Bicontinuous Donorâ€“Acceptor Ï€-Columnar Arrays in Covalent Organic Frameworks for Long-Lived Charge Separation. Journal of the American Chemical Society, 2015, 137, 7817-7827.	6.6	213
16	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
17	A Ï€-Conjugated System with Flexibility and Rigidity That Shows Environment-Dependent RGB Luminescence. Journal of the American Chemical Society, 2013, 135, 8842-8845.	6.6	191
18	Light-Emitting Covalent Organic Frameworks: Fluorescence Improving via Pinpoint Surgery and Selective Switch-On Sensing of Anions. Journal of the American Chemical Society, 2018, 140, 12374-12377.	6.6	191

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19	Sensitivity of Ammonia Interaction with Single-Walled Carbon Nanotube Bundles to the Presence of Defect Sites and Functionalities. Journal of the American Chemical Society, 2005, 127, 10533-10538.	6.6	167
20	Super-Reduced Polyoxometalates: Excellent Molecular Cluster Battery Components and Semipermeable Molecular Capacitors. Journal of the American Chemical Society, 2014, 136, 9042-9052.	6.6	162
21	Twoâ€Dimensional Tetrathiafulvalene Covalent Organic Frameworks: Towards Latticed Conductive Organic Salts. Chemistry - A European Journal, 2014, 20, 14608-14613.	1.7	147
22	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. Journal of Chemical Information and Modeling, 2020, 60, 5832-5852.	2.5	134
23	Performance of the DFTB method in comparison to DFT and semiempirical methods for geometries and energies of C20â€“C86 fullerene isomers. Chemical Physics Letters, 2005, 412, 210-216.	1.2	132
24	A New Triazineâ€Based Covalent Organic Framework for Highâ€Performance Capacitive Energy Storage. ChemSusChem, 2017, 10, 921-929.	3.6	132
25	Large pore donorâ€“acceptor covalent organic frameworks. Chemical Science, 2013, 4, 4505.	3.7	127
26	A Strap Strategy for Construction of an Excitedâ€State Intramolecular Proton Transfer (ESIPT) System with Dual Fluorescence. Angewandte Chemie - International Edition, 2014, 53, 8231-8235.	7.2	120
27	Mechanisms of Single-Walled Carbon Nanotube Nucleation, Growth, and Healing Determined Using QM/MD Methods. Accounts of Chemical Research, 2010, 43, 1375-1385.	7.6	117
28	Designed synthesis of double-stage two-dimensional covalent organic frameworks. Scientific Reports, 2015, 5, 14650.	1.6	107
29	Stacked antiaromatic porphyrins. Nature Communications, 2016, 7, 13620.	5.8	105
30	Light-melt adhesive based on dynamic carbon frameworks in a columnar liquid-crystal phase. Nature Communications, 2016, 7, 12094.	5.8	103
31	A femtomolar-range suicide germination stimulant for the parasitic plant Striga hermonthica. Science, 2018, 362, 1301-1305.	6.0	101
32	Rapid Growth of a Single-Walled Carbon Nanotube on an Iron Cluster: Density-Functional Tight-Binding Molecular Dynamics Simulations. ACS Nano, 2008, 2, 1437-1444.	7.3	98
33	Molecular Simulation of Water and Hydration Effects in Different Environments: Challenges and Developments for DFTB Based Models. Journal of Physical Chemistry B, 2014, 118, 11007-11027.	1.2	97
34	Quantum Chemical Molecular Dynamics Simulation of Single-Walled Carbon Nanotube Cap Nucleation on an Iron Particle. ACS Nano, 2009, 3, 3413-3420.	7.3	96
35	Template Effect in the Competition between Haeckelite and Graphene Growth on Ni(111): Quantum Chemical Molecular Dynamics Simulations. Journal of the American Chemical Society, 2011, 133, 18837-18842.	6.6	95
36	QM/MD Simulation of SWNT Nucleation on Transition-Metal Carbide Nanoparticles. Journal of the American Chemical Society, 2010, 132, 15699-15707.	6.6	93

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37	Insights into carbon nanotube and graphene formation mechanisms from molecular simulations: a review. Reports on Progress in Physics, 2015, 78, 036501.	8.1	93
38	Evidence for a New Twoâ€Dimensional C₄Hâ€Type Polymer Based on Hydrogenated Graphene. Advanced Materials, 2011, 23, 4497-4503.	11.1	90
39	Growth of carbon nanotubes via twisted graphene nanoribbons. Nature Communications, 2013, 4, 2548.	5.8	89
40	Comparison of Interfacial Electron Transfer through Carboxylate and Phosphonate Anchoring Groupsâ€. Journal of Physical Chemistry A, 2007, 111, 6832-6842.	1.1	88
41	Three pillars for achieving quantum mechanical molecular dynamics simulations of huge systems: Divideâ€andâ€conquer, densityâ€functional tightâ€binding, and massively parallel computation. Journal of Computational Chemistry, 2016, 37, 1983-1992.	1.5	88
42	From C2Molecules to Self-Assembled Fullerenes in Quantum Chemical Molecular Dynamics. Nano Letters, 2003, 3, 1657-1664.	4.5	87
43	Dimerization-Initiated Preferential Formation of Coronene-Based Graphene Nanoribbons in Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 15141-15145.	1.5	87
44	Density-Functional Tight-Binding Combined with the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2014, 10, 4801-4812.	2.3	87
45	Hybridization of a Flexible Cyclooctatetraene Core and Rigid Aceneimide Wings for Multiluminescent Flapping Ï€ Systems. Chemistry - A European Journal, 2014, 20, 2193-2200.	1.7	82
46	Boosting electrosynthesis of ammonia on surface-engineered MXene Ti3C2. Nano Energy, 2020, 72, 104681.	8.2	82
47	Growth of Linear Carbon Chains inside Thin Double-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2011, 115, 13166-13170.	1.5	81
48	Nearly Exclusive Growth of Small Diameter Semiconducting Single-Wall Carbon Nanotubes from Organic Chemistry Synthetic End-Cap Molecules. Nano Letters, 2015, 15, 586-595.	4.5	81
49	Origin of the size-dependent fluorescence blueshift in [n]cycloparaphenylenes. Chemical Science, 2013, 4, 187-195.	3.7	79
50	A New Porous Polymer for Highly Efficient Capacitive Energy Storage. ACS Sustainable Chemistry and Engineering, 2018, 6, 202-209.	3.2	78
51	Quantum Chemical Study of the Dissociative Adsorption of OH and H2O on Pristine and Defective Graphite (0001) Surfaces: Reaction Mechanisms and Kinetics. Journal of Physical Chemistry C, 2007, 111, 1355-1365.	1.5	77
52	Reactive Molecular Dynamics Simulation of Fullerene Combustion Synthesis: ReaxFF vs DFTB Potentials. Journal of Chemical Theory and Computation, 2011, 7, 2040-2048.	2.3	74
53	Analytical second-order geometrical derivatives of energy for the self-consistent-charge density-functional tight-binding method. Journal of Chemical Physics, 2004, 121, 5163-5170.	1.2	71
54	Cï£¿H Activation Generates Periodâ€Shortening Molecules That Target Cryptochrome in the Mammalian Circadian Clock. Angewandte Chemie - International Edition, 2015, 54, 7193-7197.	7.2	71

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55	Comparison of Geometric, Electronic, and Vibrational Properties for Isomers of Small Fullerenes C20â^'C36â€. Journal of Physical Chemistry A, 2007, 111, 6649-6657.	1.1	69
56	SWNT Nucleation from Carbon-Coated SiO₂ Nanoparticles via a Vaporâ^'Solidâ^'Solid Mechanism. Journal of the American Chemical Society, 2011, 133, 621-628.	6.6	67
57	Topologyâ€Templated Synthesis of Crystalline Porous Covalent Organic Frameworks. Angewandte Chemie - International Edition, 2020, 59, 12162-12169.	7.2	66
58	Design of tough adhesive from commodity thermoplastics through dynamic crosslinking. Science Advances, 2021, 7, eabk2451.	4.7	66
59	Directab initiovariational calculation of vibrational energies of the H2Oâ‹¯Clâ^' complex and resolution of experimental differences. Journal of Chemical Physics, 2000, 113, 8401-8403.	1.2	64
60	Zwitterionic Ladder Stilbenes with Phosphonium and Borate Bridges: Intramolecular Cascade Cyclization and Structureâ€"Photophysical Properties Relationship. Organometallics, 2011, 30, 3870-3879.	1.1	63
61	RhI-catalyzed aldol-type reaction of organonitriles under mild conditions. Chemical Communications, 2008, , 2212.	2.2	62
62	Electrically Activated Conductivity and White Light Emission of a Hydrocarbon Nanoringâ€"Iodine Assembly. Angewandte Chemie - International Edition, 2017, 56, 11196-11202.	7.2	62
63	TICT fluorescence of N-borylated 2,5-diarylpyrroles: a gear like dual motion in the excited state. Dalton Transactions, 2013, 42, 620-624.	1.6	61
64	Parametrization and Benchmark of Long-Range Corrected DFTB2 for Organic Molecules. Journal of Chemical Theory and Computation, 2018, 14, 115-125.	2.3	60
65	Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst. Journal of the American Chemical Society, 2020, 142, 7655-7667.	6.6	59
66	Defect Healing during Single-Walled Carbon Nanotube Growth: A Density-Functional Tight-Binding Molecular Dynamics Investigation. Journal of Physical Chemistry C, 2009, 113, 20198-20207.	1.5	58
67	Direct evidence of active and inactive phases of Fe catalyst nanoparticles for carbon nanotube formation. Journal of Catalysis, 2014, 319, 54-60.	3.1	57
68	A Macrocyclic Fluorophore Dimer with Flexible Linkers: Bright Excimer Emission with a Long Fluorescence Lifetime. Angewandte Chemie - International Edition, 2016, 55, 7131-7135.	7.2	55
69	Automatized Parameterization of DFTB Using Particle Swarm Optimization. Journal of Chemical Theory and Computation, 2016, 12, 53-64.	2.3	55
70	Constraint-induced structural deformation of planarized triphenylboranes in the excited state. Chemical Science, 2014, 5, 1296-1304.	3.7	54
71	Pre-Sodiated Ti₃C₂T_x MXene Structure and Behavior as Electrode for Sodium-Ion Capacitors. ACS Nano, 2021, 15, 2994-3003.	7.3	54
72	Combined ab initio and density functional study on polaron to bipolaron transitions in oligophenyls and oligothiophenes. Journal of Chemical Physics, 1997, 107, 3021-3031.	1.2	52

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73	Water Clusters on Graphite:Â Methodology for Quantum Chemical A Priori Prediction of Reaction Rate Constants. Journal of Physical Chemistry A, 2005, 109, 9563-9572.	1.1	52
74	Milestones in molecular dynamics simulations of single-walled carbon nanotube formation: A brief critical review. Nano Research, 2009, 2, 755.	5.8	52
75	Single-walled Carbon Nanotube Growth from Chiral Carbon Nanorings: Prediction of Chirality and Diameter Influence on Growth Rates. Journal of the American Chemical Society, 2012, 134, 15887-15896.	6.6	52
76	Cycloparaphenylene as a molecular porous carbon solid with uniform pores exhibiting adsorption-induced softness. Chemical Science, 2016, 7, 4204-4210.	3.7	52
77	Near infrared two-photon-excited and -emissive dyes based on a strapped excited-state intramolecular proton-transfer (ESIPT) scaffold. Chemical Science, 2018, 9, 2666-2673.	3.7	52
78	The internal coordinate path Hamiltonian; application to methanol and malonaldehyde. Molecular Physics, 2003, 101, 3513-3525.	0.8	51
79	Coupled Cluster and Density Functional Theory Calculations of Atomic Hydrogen Chemisorption on Pyrene and Coronene as Model Systems for Graphene Hydrogenation. Journal of Physical Chemistry A, 2012, 116, 7154-7160.	1.1	51
80	Formation of Fullerene Molecules from Carbon Nanotubes:Â A Quantum Chemical Molecular Dynamics Study. Nano Letters, 2003, 3, 465-470.	4.5	50
81	Substituent Effects of -NO and -NO2, Groups in Aromatic Systems. Journal of Organic Chemistry, 1995, 60, 6744-6755.	1.7	49
82	Electrical Switching Behavior of a [60]Fullereneâ€Based Molecular Wire Encapsulated in a Syndiotactic Poly(methyl methacrylate) Helical Cavity. Angewandte Chemie - International Edition, 2013, 52, 1049-1053.	7.2	49
83	Development of Smallâ€Molecule Cryptochrome Stabilizer Derivatives as Modulators of the Circadian Clock. ChemMedChem, 2015, 10, 1489-1497.	1.6	49
84	Ruthenium Nanoparticle-Decorated Porous Organic Network for Direct Hydrodeoxygenation of Long-Chain Fatty Acids to Alkanes. ACS Sustainable Chemistry and Engineering, 2018, 6, 1610-1619.	3.2	48
85	Hot Giant Fullerenes Eject and Capture C₂ Molecules: QM/MD Simulations with Constant Density. Journal of Physical Chemistry C, 2011, 115, 22707-22716.	1.5	47
86	Quantum chemical simulations reveal acetylene-based growth mechanisms in the chemical vapor deposition synthesis of carbon nanotubes. Carbon, 2014, 72, 22-37.	5.4	47
87	Quantum Chemical Molecular Dynamics Simulations of Dynamic Fullerene Self-Assembly in Benzene Combustion. ACS Nano, 2009, 3, 2241-2257.	7.3	46
88	Regioselectivity control of graphene functionalization by ripples. Physical Chemistry Chemical Physics, 2011, 13, 19449.	1.3	46
89	Anabinitioinvestigation of the chargeâ€transfer complexes of alkali atoms with oligo (Î±,Î±â€²) thiophenes and oligoparaphenylenes: A model calculation on polaronic and bipolaronic defect structures. Journal of Chemical Physics, 1995, 103, 1508-1522.	1.2	45
90	Large-Scale Quantum-Mechanical Molecular Dynamics Simulations Using Density-Functional Tight-Binding Combined with the Fragment Molecular Orbital Method. Journal of Physical Chemistry Letters, 2015, 6, 5034-5039.	2.1	45

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91	Density-functional tight-binding molecular dynamics simulations of SWCNT growth by surface carbon diffusion on an iron cluster. Carbon, 2009, 47, 1270-1275.	5.4	44
92	Hydroxide Anion Transport in Covalent Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 8970-8975.	6.6	44
93	Quantum Chemical Molecular Dynamics Model Study of Fullerene Formation from Open-Ended Carbon Nanotubesâ€. Journal of Physical Chemistry A, 2004, 108, 3182-3194.	1.1	43
94	Towards formation of buckminsterfullerene C60 in quantum chemical molecular dynamics. Journal of Chemical Physics, 2005, 122, 014708.	1.2	43
95	Comparison of single-walled carbon nanotube growth from Fe and Ni nanoparticles using quantum chemical molecular dynamics methods. Carbon, 2010, 48, 3014-3026.	5.4	42
96	Polyyne Chain Growth and Ring Collapse Drives Ni-Catalyzed SWNT Growth: A QM/MD Investigation. Journal of Physical Chemistry C, 2010, 114, 8206-8211.	1.5	42
97	Quantum chemical investigation of epoxide and ether groups in graphene oxide and their vibrational spectra. Physical Chemistry Chemical Physics, 2013, 15, 3725.	1.3	42
98	Quantum Chemical Prediction of Reaction Pathways and Rate Constants for Dissociative Adsorption of COxand NOxon the Graphite (0001) Surface. Journal of Physical Chemistry B, 2006, 110, 21135-21144.	1.2	41
99	Modeling carbon nanostructures with the self-consistent charge density-functional tight-binding method: Vibrational spectra and electronic structure of C28, C60, and C70. Journal of Chemical Physics, 2006, 125, 214706.	1.2	40
100	Temperature Dependence of Iron-Catalyzed Continued Single-Walled Carbon Nanotube Growth Rates: Density Functional Tight-Binding Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2009, 113, 159-169.	1.5	40
101	Fullerenes: formation, stability, and reactivity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 350-367.	6.2	40
102	Sub-surface nucleation of graphene precursors near a Ni(111) step-edge. Chemical Communications, 2012, 48, 7937.	2.2	40
103	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. Chemical Science, 2014, 5, 3493-3500.	3.7	40
104	Artificial neural network correction for density-functional tight-binding molecular dynamics simulations. MRS Communications, 2019, 9, 867-873.	0.8	40
105	Nucleation of Graphene Precursors on Transition Metal Surfaces: Insights from Theoretical Simulations. Journal of Physical Chemistry C, 2013, 117, 14858-14864.	1.5	39
106	Two-dimensional artificial light-harvesting antennae with predesigned high-order structure and robust photosensitising activity. Scientific Reports, 2016, 6, 32944.	1.6	39
107	Synthesis of 1â€Phosphaâ€2â€boraacenaphthenes: Reductive 1,2â€Aryl Migration of 1â€Diarylborylâ€8â€dichlorophosphinonaphthalenes. Angewandte Chemie - International Edition, 2011, 50, 10940-10943.	7.2	38
108	Dynamics of Local Chirality during SWCNT Growth: Armchair versus Zigzag Nanotubes. Journal of the American Chemical Society, 2012, 134, 9311-9319.	6.6	38

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109	Kinetic Isotope Effect in the Hydrogenation and Deuteration of Graphene. Advanced Functional Materials, 2013, 23, 1628-1635.	7.8	38
110	Origin of the Linear Relationship between CH2/NH/Oâ^'SWNT Reaction Energies and Sidewall Curvature: Armchair Nanotubes. Journal of the American Chemical Society, 2006, 128, 15117-15126.	6.6	37
111	Stochastic structure determination for conformationally flexible heterogenous molecular clusters: Application to ionic liquids. Journal of Computational Chemistry, 2013, 34, 2591-2600.	1.5	37
112	Third-order density-functional tight-binding combined with the fragment molecular orbital method. Chemical Physics Letters, 2015, 636, 90-96.	1.2	37
113	Dipole moments of highly vibrationally excited HCN: Theoretical prediction of an experimental diagnostic for delocalized states. Journal of Chemical Physics, 2001, 114, 7923-7934.	1.2	36
114	Quantum Chemical Molecular Dynamics Study of "Shrinking" of Hot Giant Fullerenes. Journal of Nanoscience and Nanotechnology, 2007, 7, 1662-1669.	0.9	36
115	Convergence in the Evolution of Nanodiamond Raman Spectra with Particle Size: A Theoretical Investigation. ACS Nano, 2010, 4, 4475-4486.	7.3	36
116	Dramatic Reduction of IR Vibrational Cross Sections of Molecules Encapsulated in Carbon Nanotubes. Journal of the American Chemical Society, 2011, 133, 8191-8198.	6.6	36
117	Fabrication and Optical Probing of Highly Extended, Ultrathin Graphene Nanoribbons in Carbon Nanotubes. ACS Nano, 2015, 9, 5034-5040.	7.3	36
118	The Fragment Molecular Orbital Method Based on Long-Range Corrected Density-Functional Tight-Binding. Journal of Chemical Theory and Computation, 2019, 15, 3008-3020.	2.3	35
119	Theoretical Study of Structure and Raman Spectra for Models of Carbon Nanotubes in Their Pristine and Oxidized Forms. Journal of Physical Chemistry A, 2002, 106, 11973-11980.	1.1	34
120	A Ï€-stacked phenylacetylene dimer. Physical Chemistry Chemical Physics, 2011, 13, 16706.	1.3	33
121	Substituent Effects on Twisted Internal Charge Transfer Excited States of N-Borylated Carbazoles and (Diphenylamino)boranes. Journal of Physical Chemistry A, 2012, 116, 1151-1158.	1.1	33
122	Quantum Dynamics Simulations Reveal Vibronic Effects on the Optical Properties of [n]Cycloparaphenylenes. Journal of Chemical Theory and Computation, 2014, 10, 4025-4036.	2.3	32
123	Molecular dynamics simulation of hydrogen atom sputtering on the surface of graphite with defect and edge. Journal of Nuclear Materials, 2009, 390-391, 183-187.	1.3	31
124	Interaction of Acetone with Single Wall Carbon Nanotubes at Cryogenic Temperatures: A Combined Temperature Programmed Desorption and Theoretical Study. Langmuir, 2008, 24, 7848-7856.	1.6	30
125	Single-walled carbon nanotube growth from a cap fragment on an iron nanoparticle: Density-functional tight-binding molecular dynamics simulations. Physical Review B, 2009, 79, .	1.1	30
126	Collision-induced fusion of twoC60fullerenes: Quantum chemical molecular dynamics simulations. Physical Review B, 2010, 82, .	1.1	30

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127	Simulations of the synthesis of boron-nitride nanostructures in a hot, high pressure gas volume. Chemical Science, 2018, 9, 3803-3819.	3.7	28
128	ONIOM Study of Ring Opening and Metal Insertion Reactions with Derivatives of C60:â€‰ Role of Aromaticity in the Opening Process. Journal of Physical Chemistry A, 2002, 106, 680-688.	1.1	27
129	Quantum Chemical Prediction of Pathways and Rate Constants for Reactions of CO and CO2 with Vacancy Defects on Graphite (0001) Surfaces. Journal of Physical Chemistry C, 2009, 113, 18772-18777.	1.5	27
130	Theoretical Insights into Chiralityâ€Controlled SWCNT Growth from a Cycloparaphenylene Template. ChemPhysChem, 2012, 13, 1479-1485.	1.0	26
131	Graphene Nucleation from Amorphous Nickel Carbides: QM/MD Studies on the Role of Subsurface Carbon Density. Journal of Physical Chemistry C, 2014, 118, 11078-11084.	1.5	26
132	Theoretical study of cellobiose hydrolysis to glucose in ionic liquids. Chemical Physics Letters, 2014, 603, 7-12.	1.2	26
133	Self-assembly of endohedral metallofullerenes: a decisive role of cooling gas and metalâ€“carbon bonding. Nanoscale, 2016, 8, 3796-3808.	2.8	26
134	Polymorphism of [6]Cycloparaphenylene for Packing Structure-dependent Hostâ€“Guest Interaction. Chemistry Letters, 2017, 46, 855-857.	0.7	26
135	Formation mechanism of polycyclic aromatic hydrocarbons in benzene combustion: Quantum chemical molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 224303.	1.2	25
136	Quantum Chemical Simulation of Carbon Nanotube Nucleation on Al2O3 Catalysts via CH4 Chemical Vapor Deposition. Journal of the American Chemical Society, 2015, 137, 9281-9288.	6.6	25
137	Theoretical Investigation of the Structures and Dynamics of Crystalline Molecular Gyroscopes. Journal of Physical Chemistry C, 2012, 116, 24845-24854.	1.5	24
138	Atom-by-atom simulations of graphene growth by decomposition of SiC (0001): Impact of the substrate steps. Applied Physics Letters, 2013, 103, 141602.	1.5	24
139	Step-edge self-assembly during graphene nucleation on a nickel surface: QM/MD simulations. Nanoscale, 2014, 6, 140-144.	2.8	24
140	Glucose transformation to 5â€hydroxymethylfurfural in acidic ionic liquid: A quantum mechanical study. Journal of Computational Chemistry, 2016, 37, 327-335.	1.5	24
141	Modeling Charge Transfer in Fullerene Collisions via Real-Time Electron Dynamics. Journal of Physical Chemistry Letters, 2012, 3, 1536-1542.	2.1	23
142	Water-mediated deracemization of a bisporphyrin helicate assisted by diastereoselective encapsulation of chiral guests. Nature Communications, 2019, 10, 1457.	5.8	23
143	An ab initio study of the vibrational spectra of Li-doped thiophene, bithiophene, benzene and biphenyl as model systems for (bi)polaronic defects. Computational and Theoretical Chemistry, 1996, 364, 15-31.	1.5	22
144	A Macrocyclic Fluorophore Dimer with Flexible Linkers: Bright Excimer Emission with a Long Fluorescence Lifetime. Angewandte Chemie, 2016, 128, 7247-7251.	1.6	22

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145	Cryptic bioactivity capacitated by synthetic hybrid plant peptides. Nature Communications, 2017, 8, 14318.	5.8	22
146	Theory and experiment agree: Single-walled carbon nanotube caps grow catalyst-free with chirality preference on a SiC surface. Journal of Chemical Physics, 2006, 125, 044702.	1.2	21
147	Carbon Nanotubes Grow on the C Face of SiC (0001Ì„) during Sublimation Decomposition:â€‰ Quantum Chemical Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2007, 111, 12960-12972.	1.5	21
148	Delocalization errors in a hubbardâ€like model: Consequences for densityâ€functional tightâ€binding calculations of molecular systems. International Journal of Quantum Chemistry, 2012, 112, 1701-1711.	1.0	21
149	Comparison of geometric, electronic, and vibrational properties for all pentagon/hexagonâ€bearing isomers of fullerenes C₃₈, C₄₀, and C₄₂. International Journal of Quantum Chemistry, 2009, 109, 1999-2011.	1.0	20
150	Structure of Tm2 and Tm2C2 encapsulated in low-symmetry C82(Cs(6)) fullerene cage by single crystal X-ray diffraction. Chemical Physics Letters, 2014, 600, 38-42.	1.2	20
151	QM/MD studies on graphene growth from small islands on the Ni(111) surface. Nanoscale, 2016, 8, 3067-3074.	2.8	20
152	Topologyâ€Templated Synthesis of Crystalline Porous Covalent Organic Frameworks. Angewandte Chemie, 2020, 132, 12260-12267.	1.6	20
153	Temperature and pressure dependence of molecular adsorption on single wall carbon nanotubes and the existence of an â€œadsorption/desorption pressure gapâ€. Carbon, 2010, 48, 1867-1875.	5.4	19
154	Density-functional tight-binding for phosphine-stabilized nanoscale gold clusters. Chemical Science, 2020, 11, 13113-13128.	3.7	19
155	Strain-Induced Growth of Twisted Bilayers during the Coalescence of Monolayer MoS₂ Crystals. ACS Nano, 2021, 15, 4504-4517.	7.3	19
156	Relative Isomer Abundance of Fullerenes and Carbon Nanotubes Correlates with Kinetic Stability. Physical Review Letters, 2011, 107, 175506.	2.9	18
157	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.	2.3	18
158	A molecular orbital study on H and H2 elimination pathways from methane, ethane, and propane. Journal of Chemical Physics, 2000, 113, 6139-6148.	1.2	17
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