Stephan Irle

List of Publications by Year
in descending order

277 papers	14,688 citations	19657 61 h-index	24982 109 g-index
305 all docs	305 docs citations	305 times ranked	14404 citing authors

#	Article	IF	Citations
1	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
2	Dynamic aspects of graphene deformation and fracture from approximate density functional theory. Carbon, 2022, 190, 183-193.	10.3	8
3	The FMO-DFTB Method. , 2021, , 459-485.		4
4	How the Size and Density of Charge-Transfer Excitons Depend on Heterojunctionâ€™s Architecture. Journal of Physical Chemistry C, 2021, 125, 5458-5474.	3.1	6
5	Strain-Induced Growth of Twisted Bilayers during the Coalescence of Monolayer MoS₂ Crystals. ACS Nano, 2021, 15, 4504-4517.	14.6	19
6	Density-Functional Tight-Binding Parameters for Bulk Zirconium: A Case Study for Repulsive Potentials. Journal of Physical Chemistry A, 2021, 125, 2184-2196.	2.5	2
7	Hydroxide Anion Transport in Covalent Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 8970-8975.	13.7	44
8	Development of Density-Functional Tight-Binding Parameters for the Molecular Dynamics Simulation of Zirconia, Yttria, and Yttria-Stabilized Zirconia. ACS Omega, 2021, 6, 20530-20548.	3.5	8
9	Density Functional Tight-Binding Simulations Reveal the Presence of Surface Defects on the Quartz (101)â€“Water Interface. Journal of Physical Chemistry C, 2021, 125, 16246-16255.	3.1	4
10	Encapsulation of Aromatic Guests in the Bisporphyrin Cavity of a Double-Stranded Spiroborate Helicate: Thermodynamic and Kinetic Studies and the Encapsulation Mechanism. Journal of Organic Chemistry, 2021, 86, 10501-10516.	3.2	5
11	Methane Adsorption on Heteroatom-ModifiedMaquettesof Porous Carbon Surfaces. Journal of Physical Chemistry A, 2021, 125, 6042-6058.	2.5	5
12	Investigating the Accuracy of Water Models through the Van Hove Correlation Function. Journal of Chemical Theory and Computation, 2021, 17, 5992-6005.	5.3	9
13	Pre-Sodiated Ti₃C₂T_x MXene Structure and Behavior as Electrode for Sodium-Ion Capacitors. ACS Nano, 2021, 15, 2994-3003.	14.6	54
14	Design of tough adhesive from commodity thermoplastics through dynamic crosslinking. Science Advances, 2021, 7, eabk2451.	10.3	66
15	Density-functional tight-binding for phosphine-stabilized nanoscale gold clusters. Chemical Science, 2020, 11, 13113-13128.	7.4	19
16	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. Journal of Chemical Information and Modeling, 2020, 60, 5832-5852.	5.4	134
17	Boosting electrosynthesis of ammonia on surface-engineered MXene Ti3C2. Nano Energy, 2020, 72, 104681.	16.0	82
18	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589

#	Article	IF	Citations
19	Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst. Journal of the American Chemical Society, 2020, 142, 7655-7667.	13.7	59
20	Topologyâ€Templated Synthesis of Crystalline Porous Covalent Organic Frameworks. Angewandte Chemie - International Edition, 2020, 59, 12162-12169.	13.8	66
21	Topologyâ€Templated Synthesis of Crystalline Porous Covalent Organic Frameworks. Angewandte Chemie, 2020, 132, 12260-12267.	2.0	20
22	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
23	Protein Molecular Dynamics Simulations with Approximate QM: What Can We Learn?. Methods in Molecular Biology, 2020, 2114, 149-161.	0.9	2
24	Artificial neural network correction for density-functional tight-binding molecular dynamics simulations. MRS Communications, 2019, 9, 867-873.	1.8	40
25	The helixâ€inversion mechanism in doubleâ€stranded helical oligomers bridged by rotary cyclic boronate esters. Journal of Computational Chemistry, 2019, 40, 2036-2042.	3.3	0
26	The Fragment Molecular Orbital Method Based on Long-Range Corrected Density-Functional Tight-Binding. Journal of Chemical Theory and Computation, 2019, 15, 3008-3020.	5.3	35
27	Phenyleneethynylene trimer-based rigid-flexible [2+2] macrocycles for nucleic acid labelling in live cells. Chemical Communications, 2019, 55, 5930-5933.	4.1	11
28	Structural transformations of graphene exposed to nitrogen plasma: quantum chemical molecular dynamics simulations. Physical Chemistry Chemical Physics, 2019, 21, 12112-12120.	2.8	9
29	Water-mediated deracemization of a bisporphyrin helicate assisted by diastereoselective encapsulation of chiral guests. Nature Communications, 2019, 10, 1457.	12.8	23
30	How does acetonitrile modulate single-walled carbon nanotube diameter during CVD growth?. Carbon, 2019, 146, 535-541.	10.3	11
31	Nonadiabatic excited-state intramolecular proton transfer in 3-hydroxyflavone: S2 state involvement via multi-mode effect. Journal of Chemical Physics, 2019, 151, 214304.	3.0	9
32	Density-Functional Tight-Binding for Platinum Clusters and Bulk: Electronic vs Repulsive Parameters. MRS Advances, 2019, 4, 1821-1832.	0.9	3
33	Chiralâ€selective etching effects on carbon nanotube growth at edge carbon atoms. Journal of Computational Chemistry, 2019, 40, 375-380.	3.3	5
34	Low-energy hydrogen uptake by small-cage Cn and Cn-1B fullerenes. Carbon, 2018, 134, 189-198.	10.3	17
35	Keiji Morokuma (1934â€“2017). Angewandte Chemie - International Edition, 2018, 57, 2288-2289.	13.8	0
36	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.	7.4	52

#	Article	IF	Citations
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	A New Porous Polymer for Highly Efficient Capacitive Energy Storage. ACS Sustainable Chemistry and Engineering, 2018, 6, 202-209.	6.7	78
39	Simulations of the synthesis of boron-nitride nanostructures in a hot, high pressure gas volume. Chemical Science, 2018, 9, 3803-3819.	7.4	28
40	Implementation of replica-exchange umbrella sampling in GAMESS. Computer Physics Communications, 2018, 228, 152-162.	7.5	10
41	Conformational dynamics of human protein kinase CK2Î± and its effect on function and inhibition. Proteins: Structure, Function and Bioinformatics, 2018, 86, 344-353.	2.6	8
42	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.	6.7	48
43	Statistical Mechanics-Based Theoretical Investigation of Solvation Effects on Glucose Anomer Preferences. Journal of Physical Chemistry B, 2018, 122, 290-296.	2.6	5
44	A femtomolar-range suicide germination stimulant for the parasitic plant Striga hermonthica. Science, 2018, 362, 1301-1305.	12.6	101
45	Performance of Density-Functional Tight-Binding in Comparison to Ab Initio and First-Principles Methods for Isomer Geometries and Energies of Glucose Epimers in Vacuo and Solution. ACS Omega, 2018, 3, 16899-16915.	3.5	12
46	When finite becomes infinite: convergence properties of vibrational spectra of oligomer chains. Journal of Molecular Modeling, 2018, 24, 288.	1.8	5
47	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.	13.7	191
48	Theoretical Prediction and Analysis of the UV/Visible Absorption and Emission Spectra of Chiral Carbon Nanorings. Journal of Physical Chemistry A, 2018, 122, 7284-7292.	2.5	8
49	Theoretical analysis of orientations and tautomerization of genistein in Î²-cyclodextrin. Journal of Molecular Liquids, 2018, 265, 16-23.	4.9	11
50	Quantum chemical replica-exchange umbrella sampling molecular dynamics simulations reveal the formation mechanism of iron phthalocyanine from iron and phthalonitrile. Journal of Chemical Physics, 2018, 149, 072332.	3.0	1
51	Decoding Oxyanion Aqueous Solvation Structure: A Potassium Nitrate Example at Saturation. Journal of Physical Chemistry B, 2018, 122, 7584-7589.	2.6	14
52	Focus-Induced Photoresponse: a novel way to measure distances with photodetectors. Scientific Reports, 2018, 8, 9208.	3.3	16
53	Inducing regioselective chemical reactivity in graphene with alkali metal intercalation. Physical Chemistry Chemical Physics, 2018, 20, 19987-19994.	2.8	6
54	A New Triazineâ€Based Covalent Organic Framework for Highâ€Performance Capacitive Energy Storage. ChemSusChem, 2017, 10, 921-929.	6.8	132

#	Article	IF	Citations
55	Theoretical Studies on Ethanol Dissociation on Iron Nanoparticles in the Early Stage of SWCNT Growth. Journal of Physical Chemistry C, 2017, 121, 2276-2284.	3.1	16
56	FÃ¶rster Resonance Energy Transfer between Fluorescent Proteins: Efficient Transition Charge-Based Study. Journal of Physical Chemistry C, 2017, 121, 4220-4238.	3.1	11
57	Cryptic bioactivity capacitated by synthetic hybrid plant peptides. Nature Communications, 2017, 8, 14318.	12.8	22
58	Theoretical rationalization for reduced charge recombination in bulky carbazoleâ€based sensitizers in solar cells. Journal of Computational Chemistry, 2017, 38, 901-909.	3.3	2
59	Doubleâ€Stranded Helical Oligomers Covalently Bridged by Rotary Cyclic Boronate Esters. Chemistry - an Asian Journal, 2017, 12, 927-935.	3.3	15
60	Theoretical Elucidation of Potential Enantioselectivity in a Pd-Catalyzed Aromatic Câ€“H Coupling Reaction. Journal of Organic Chemistry, 2017, 82, 4900-4906.	3.2	13
61	QM/MD Simulations on Graphene Hydrogenation/Deuteration: C_xH/D Formation Mechanism and Isotope Effect. Journal of Physical Chemistry C, 2017, 121, 8480-8489.	3.1	2
62	Quantum Chemical Estimation of Acetone Physisorption on Graphene Using Combined Basis Set and Size Extrapolation Schemes. Journal of Physical Chemistry C, 2017, 121, 8999-9010.	3.1	5
63	Coupled Cluster and Density Functional Studies of Atomic Fluorine Chemisorption on Coronene as Model Systems for Graphene Fluorination. Journal of Physical Chemistry C, 2017, 121, 14888-14898.	3.1	12
64	Importance of oxygen in single-walled carbon nanotube growth: Insights from QM/MD simulations. Carbon, 2017, 121, 292-300.	10.3	10
65	Electrically Activated Conductivity and White Light Emission of a Hydrocarbon Nanoringâ€“Iodine Assembly. Angewandte Chemie, 2017, 129, 11348-11354.	2.0	17
66	Er³⁺ Photoluminescence in Er₂@C₈₂ and Er₂C₂@C₈₂ Metallofullerenes Elucidated by Density Functional Theory. Inorganic Chemistry, 2017, 56, 6576-6583.	4.0	10
67	Quantum chemical molecular dynamics simulation of carbon nanotubeâ€“graphene fusion. Molecular Simulation, 2017, 43, 1269-1276.	2.0	5
68	Constructing Sulfonic Acid Functionalized Anthracene Derived Conjugated Porous Organic Polymer for Efficient Metal-Free Catalytic Acetalization of Bio-Glycerol. ChemistrySelect, 2017, 2, 4705-4716.	1.5	15
69	Polymorphism of [6]Cycloparaphenylene for Packing Structure-dependent Hostâ€“Guest Interaction. Chemistry Letters, 2017, 46, 855-857.	1.3	26
70	Structural influence of transition metal (Sc, Y, and Lu) atoms inside gold nanoparticles. International Journal of Quantum Chemistry, 2017, 117, e25371.	2.0	3
71	Indirect Intersystem Crossing (S1 â†' T3/T2 â†' T1) Promoted by the Jahnâ€“Teller Effect in Cycloparaphenylenes. Journal of Chemical Theory and Computation, 2017, 13, 4944-4949.	5.3	7
72	Multiscale Simulations on Charge Transport in Covalent Organic Frameworks Including Dynamics of Transfer Integrals from the FMO-DFTB/LCMO Approach. Journal of Physical Chemistry C, 2017, 121, 17712-17726.	3.1	16

#	Article	IF	Citations
73	Unraveling the plasma-material interface with real time diagnosis of dynamic boron conditioning in extreme tokamak plasmas. Nuclear Fusion, 2017, 57, 086050.	3.5	11
74	Development of density-functional tight-binding repulsive potentials for bulk zirconia using particle swarm optimization algorithm. AIP Conference Proceedings, 2017, , .	0.4	3
75	Quantum chemical prediction of vibrational spectra of large molecular systems with radical or metallic electronic structure. Chemical Physics Letters, 2017, 667, 317-321.	2.6	7
76	Electrically Activated Conductivity and White Light Emission of a Hydrocarbon Nanoringâ€“Iodine Assembly. Angewandte Chemie - International Edition, 2017, 56, 11196-11202.	13.8	62
77	Ab initio and first principles theoretical investigations of tripletâ€“triplet fluorescence in trimethylenemethane biradicals. RSC Advances, 2016, 6, 83668-83672.	3.6	3
78	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.	3.3	88
79	Glucose transformation to 5â€hydroxymethylfurfural in acidic ionic liquid: A quantum mechanical study. Journal of Computational Chemistry, 2016, 37, 327-335.	3.3	24
80	A Macrocyclic Fluorophore Dimer with Flexible Linkers: Bright Excimer Emission with a Long Fluorescence Lifetime. Angewandte Chemie - International Edition, 2016, 55, 7131-7135.	13.8	55
81	A Macrocyclic Fluorophore Dimer with Flexible Linkers: Bright Excimer Emission with a Long Fluorescence Lifetime. Angewandte Chemie, 2016, 128, 7247-7251.	2.0	22
82	A global reaction route mapping-based kinetic Monte Carlo algorithm. Journal of Chemical Physics, 2016, 145, 024105.	3.0	12
83	Molecular dynamics in computational materials sciences: From the study of nanostructure formation to the design of fluorescent dyes. AIP Conference Proceedings, 2016, , .	0.4	0
84	Theoretical Investigation of Molecular and Electronic Structures of Buckminsterfullerene-Silicon Quantum Dot Systems. Journal of Physical Chemistry A, 2016, 120, 9767-9775.	2.5	2
85	Stacked antiaromatic porphyrins. Nature Communications, 2016, 7, 13620.	12.8	105
86	Molecular dynamical modelling of endohedral fullerenes formation in plasma. IOP Conference Series: Materials Science and Engineering, 2016, 110, 012078.	0.6	0
87	Implementation of replica-exchange umbrella sampling in the DFTB<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si6.gif" display="inline" overflow="scroll"><mml:mo>+</mml:mo></mml:math> semiempirical quantum chemistry package. Computer Physics Communications, 2016, 204, 1-10.	7.5	6
88	Understanding of the Offâ€“On Response Mechanism in Caged Fluorophores Based on Quantum and Statistical Mechanics. Journal of Physical Chemistry B, 2016, 120, 4449-4456.	2.6	9
89	Theoretical analysis of structural diversity of covalent organic framework: Stacking isomer structures thermodynamics and kinetics. Chemical Physics Letters, 2016, 664, 101-107.	2.6	13
90	Chiral-Selective Carbon Nanotube Etching with Ammonia: A Quantum Chemical Investigation. Journal of Physical Chemistry C, 2016, 120, 19862-19870.	3.1	7

#	Article	IF	Citations
91	Light-melt adhesive based on dynamic carbon frameworks in a columnar liquid-crystal phase. Nature Communications, 2016, 7, 12094.	12.8	103
92	Two-dimensional artificial light-harvesting antennae with predesigned high-order structure and robust photosensitising activity. Scientific Reports, 2016, 6, 32944.	3.3	39
93	Spanning the â€œParameter Spaceâ€•of Chemical Vapor Deposition Graphene Growth with Quantum Chemical Simulations. Journal of Physical Chemistry C, 2016, 120, 13851-13864.	3.1	14
94	QM/MD studies on graphene growth from small islands on the Ni(111) surface. Nanoscale, 2016, 8, 3067-3074.	5.6	20
95	Self-assembly of endohedral metallofullerenes: a decisive role of cooling gas and metalâ€“carbon bonding. Nanoscale, 2016, 8, 3796-3808.	5.6	26
96	Self-Consistent Optimization of Excited States within Density-Functional Tight-Binding. Journal of Chemical Theory and Computation, 2016, 12, 313-323.	5.3	11
97	Automatized Parameterization of DFTB Using Particle Swarm Optimization. Journal of Chemical Theory and Computation, 2016, 12, 53-64.	5.3	55
98	Automatized Parameterization of the Densityâ€functional Tightâ€binding Method. II. Twoâ€center Integrals. Journal of the Chinese Chemical Society, 2016, 63, 57-68.	1.4	13
99	Diversity in electronic structure and vibrational properties of fullerene isomers correlates with cage curvature. Carbon, 2016, 100, 484-491.	10.3	10
100	Cycloparaphenylene as a molecular porous carbon solid with uniform pores exhibiting adsorption-induced softness. Chemical Science, 2016, 7, 4204-4210.	7.4	52
101	Understanding the Onâ€“Off Switching Mechanism in Cationic Tetravalent Group-V-Based Fluoride Molecular Sensors Using Orbital Analysis. Journal of Physical Chemistry A, 2015, 119, 12693-12698.	2.5	12
102	Implementation of Replica-Exchange Umbrella Sampling to the DFTB+ Simulation Package. Biophysical Journal, 2015, 108, 159a.	0.5	0
103	RÃ¼cktitelbild: Cï£¿H Activation Generates Period-Shortening Molecules That Target Cryptochrome in the Mammalian Circadian Clock (Angew. Chem. 24/2015). Angewandte Chemie, 2015, 127, 7306-7306.	2.0	0
104	Designed synthesis of double-stage two-dimensional covalent organic frameworks. Scientific Reports, 2015, 5, 14650.	3.3	107
105	A Benzophosphole P-Oxide with an Electron-Donating Group at 3-Position: Enhanced Fluorescence in Polar Solvents. Bulletin of the Chemical Society of Japan, 2015, 88, 1545-1552.	3.2	15
106	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.	13.7	213
107	Development of Smallâ€Molecule Cryptochrome Stabilizer Derivatives as Modulators of the Circadian Clock. ChemMedChem, 2015, 10, 1489-1497.	3.2	49
108	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.	13.7	320

#	Article	IF	Citations
109	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.	13.7	25
110	Rational design of crystalline supermicroporous covalent organic frameworks with triangular topologies. Nature Communications, 2015, 6, 7786.	12.8	274
111	Fabrication and Optical Probing of Highly Extended, Ultrathin Graphene Nanoribbons in Carbon Nanotubes. ACS Nano, 2015, 9, 5034-5040.	14.6	36
112	Cï£¿H Activation Generates Periodâ€Shortening Molecules That Target Cryptochrome in the Mammalian Circadian Clock. Angewandte Chemie, 2015, 127, 7299-7303.	2.0	4
113	Cï£¿H Activation Generates Periodâ€Shortening Molecules That Target Cryptochrome in the Mammalian Circadian Clock. Angewandte Chemie - International Edition, 2015, 54, 7193-7197.	13.8	71
114	Insights into carbon nanotube and graphene formation mechanisms from molecular simulations: a review. Reports on Progress in Physics, 2015, 78, 036501.	20.1	93
115	Third-order density-functional tight-binding combined with the fragment molecular orbital method. Chemical Physics Letters, 2015, 636, 90-96.	2.6	37
116	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.	4.6	45
117	Nearly Exclusive Growth of Small Diameter Semiconducting Single-Wall Carbon Nanotubes from Organic Chemistry Synthetic End-Cap Molecules. Nano Letters, 2015, 15, 586-595.	9.1	81
118	Key Structures and Interactions for Binding of Mycobacterium tuberculosis Protein Kinase B Inhibitors from Molecular Dynamics Simulation. Chemical Biology and Drug Design, 2015, 86, 91-101.	3.2	2
119	Back Cover: Theoretical investigation of molecular and electronic structure changes of the molecular magnet Mn₁₂ cluster upon superâ€reduction (Phys. Status Solidi RRL 6/2014). Physica Status Solidi - Rapid Research Letters, 2014, 8, .	2.4	0
120	Theoretical investigation of molecular and electronic structure changes of the molecular magnet Mn₁₂ cluster upon superâ€reduction. Physica Status Solidi - Rapid Research Letters, 2014, 8, 517-521.	2.4	3
121	Critical interpretation of CHâ€“ and OHâ€“ stretching regions for infrared spectra of methanol clusters (CH3OH)n (n = 2â€“5) using self-consistent-charge density functional tight-binding molecular dynamics simulations. Journal of Chemical Physics, 2014, 141, 094303.	3.0	17
122	Growth mechanisms and selectivity for graphene or carbon nanotube formation on SiC (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.6	8
123	Nonequilibrium quantum chemical molecular dynamics simulations of C60 to SiC heterofullerene conversion. Carbon, 2014, 68, 285-295.	10.3	13
124	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.	2.6	20
125	Quantum chemical simulations reveal acetylene-based growth mechanisms in the chemical vapor deposition synthesis of carbon nanotubes. Carbon, 2014, 72, 22-37.	10.3	47
126	Hybridization of a Flexible Cyclooctatetraene Core and Rigid Aceneimide Wings for Multiluminescent Flapping Ï€ Systems. Chemistry - A European Journal, 2014, 20, 2193-2200.	3.3	82

#	Article	IF	Citations
127	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.	3.1	26
128	Constraint-induced structural deformation of planarized triphenylboranes in the excited state. Chemical Science, 2014, 5, 1296-1304.	7.4	54
129	Step-edge self-assembly during graphene nucleation on a nickel surface: QM/MD simulations. Nanoscale, 2014, 6, 140-144.	5.6	24
130	Density-Functional Tight-Binding Combined with the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2014, 10, 4801-4812.	5.3	87
131	Catalytic covalent organic frameworks via pore surface engineering. Chemical Communications, 2014, 50, 1292-1294.	4.1	292
132	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.	2.6	97
133	Quantum Dynamics Simulations Reveal Vibronic Effects on the Optical Properties of [n]Cycloparaphenylenes. Journal of Chemical Theory and Computation, 2014, 10, 4025-4036.	5.3	32
134	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. Chemical Science, 2014, 5, 3493-3500.	7.4	40
135	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.	13.8	120
136	Direct evidence of active and inactive phases of Fe catalyst nanoparticles for carbon nanotube formation. Journal of Catalysis, 2014, 319, 54-60.	6.2	57
137	Theoretical study of cellobiose hydrolysis to glucose in ionic liquids. Chemical Physics Letters, 2014, 603, 7-12.	2.6	26
138	Twoâ€Dimensional Tetrathiafulvalene Covalent Organic Frameworks: Towards Latticed Conductive Organic Salts. Chemistry - A European Journal, 2014, 20, 14608-14613.	3.3	147
139	Super-Reduced Polyoxometalates: Excellent Molecular Cluster Battery Components and Semipermeable Molecular Capacitors. Journal of the American Chemical Society, 2014, 136, 9042-9052.	13.7	162
140	Elucidating the structural basis of diphenyl ether derivatives as highly potent enoyl-ACP reductase inhibitors through molecular dynamics simulations and 3D-QSAR study. Journal of Molecular Modeling, 2014, 20, 2319.	1.8	5
141	Stochastic structure determination for conformationally flexible heterogenous molecular clusters: Application to ionic liquids. Journal of Computational Chemistry, 2013, 34, 2591-2600.	3.3	37
142	Photochemical Double 5â€exo Cyclization of Alkenylâ€Substituted Dithienylacetylenes: Efficient Synthesis of Diarylated Dithienofulvalenes. Angewandte Chemie - International Edition, 2013, 52, 10519-10523.	13.8	13
143	Temperature Dependence of Catalyst-Free Chirality-Controlled Single-Walled Carbon Nanotube Growth from Organic Templates. Journal of Physical Chemistry Letters, 2013, 4, 3176-3180.	4.6	11
144	Conjugated organic framework with three-dimensionally ordered stable structure and delocalized Ï€ clouds. Nature Communications, 2013, 4, 2736.	12.8	528

#	Article	IF	Citations
145	Atom-by-atom simulations of graphene growth by decomposition of SiC (0001): Impact of the substrate steps. Applied Physics Letters, 2013, 103, 141602.	3.3	24
146	Revealing the Dual Role of Hydrogen for Growth Inhibition and Defect Healing in Polycyclic Aromatic Hydrocarbon Formation: QM/MD Simulations. Journal of Physical Chemistry Letters, 2013, 4, 2323-2327.	4.6	17
147	Carbon Coating Precedes SWCNT Nucleation on Silicon Nanoparticles: Insights from QM/MD Simulations. Journal of Physical Chemistry C, 2013, 117, 4238-4244.	3.1	11
148	Large pore donorâ€“acceptor covalent organic frameworks. Chemical Science, 2013, 4, 4505.	7.4	127
149	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.	13.7	257
150	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.	13.8	49
151	Quantum chemical investigation of epoxide and ether groups in graphene oxide and their vibrational spectra. Physical Chemistry Chemical Physics, 2013, 15, 3725.	2.8	42
152	Origin of the size-dependent fluorescence blueshift in [n]cycloparaphenylenes. Chemical Science, 2013, 4, 187-195.	7.4	79
153	High-temperature transformation of Fe-decorated single-wall carbon nanohorns to nanooysters: a combined experimental and theoretical study. Nanoscale, 2013, 5, 1849-1857.	5.6	10
154	Charge Dynamics in A Donorâ€“Acceptor Covalent Organic Framework with Periodically Ordered Bicontinuous Heterojunctions. Angewandte Chemie - International Edition, 2013, 52, 2017-2021.	13.8	263
155	TICT fluorescence of N-borylated 2,5-diarylpyrroles: a gear like dual motion in the excited state. Dalton Transactions, 2013, 42, 620-624.	3.3	61
156	Nucleation of Graphene Precursors on Transition Metal Surfaces: Insights from Theoretical Simulations. Journal of Physical Chemistry C, 2013, 117, 14858-14864.	3.1	39
157	A Ï€-Conjugated System with Flexibility and Rigidity That Shows Environment-Dependent RGB Luminescence. Journal of the American Chemical Society, 2013, 135, 8842-8845.	13.7	191
158	Kinetic Isotope Effect in the Hydrogenation and Deuteration of Graphene. Advanced Functional Materials, 2013, 23, 1628-1635.	14.9	38
159	Growth of carbon nanotubes via twisted graphene nanoribbons. Nature Communications, 2013, 4, 2548.	12.8	89
160	Stochastic Search of Molecular Cluster Interaction Energy Surfaces with Coupled Cluster Quality Prediction. The Phenylacetylene Dimer. Journal of Chemical Theory and Computation, 2013, 9, 3848-3854.	5.3	2
161	Atomistic Mechanism of Carbon Nanostructure Self-Assembly as Predicted by Nonequilibrium QM/MD Simulations. , 2012, , 103-172.		5
162	Optimization of density functional tight-binding and classical reactive molecular dynamics for high-throughput simulations of carbon materials. , 2012, , .		1

#	Article	IF	Citations
163	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.	13.7	385
164	Sub-surface nucleation of graphene precursors near a Ni(111) step-edge. Chemical Communications, 2012, 48, 7937.	4.1	40
165	Optimization of a Genetic Algorithm for the Functionalization of Fullerenes. Journal of Chemical Theory and Computation, 2012, 8, 1841-1851.	5.3	14
166	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.	2.5	33
167	Theoretical Investigation of the Structures and Dynamics of Crystalline Molecular Gyroscopes. Journal of Physical Chemistry C, 2012, 116, 24845-24854.	3.1	24
168	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.	13.7	52
169	Effects of Molecular Dynamics Thermostats on Descriptions of Chemical Nonequilibrium. Journal of Chemical Theory and Computation, 2012, 8, 4019-4028.	5.3	16
170	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.	2.5	51
171	Modeling Charge Transfer in Fullerene Collisions via Real-Time Electron Dynamics. Journal of Physical Chemistry Letters, 2012, 3, 1536-1542.	4.6	23
172	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.	2.0	21
173	Molecular and electronic structures of endohedral fullerenes, Sc₂C₂@C_{3v}â€“C₈₂ and Sc₂@C_{3v}â€“C₈₂: Benchmark for SCCâ€DFTB and proposal of new inner cluster structures. Physica Status Solidi (B): Basic Research, 2012, 249, 324-334.	1.5	15
174	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.	13.8	344
175	Dimerization-Initiated Preferential Formation of Coronene-Based Graphene Nanoribbons in Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 15141-15145.	3.1	87
176	An Ambipolar Conducting Covalent Organic Framework with Selfâ€Sorted and Periodic Electron Donorâ€Acceptor Ordering. Advanced Materials, 2012, 24, 3026-3031.	21.0	258
177	Theoretical Insights into Chiralityâ€Controlled SWCNT Growth from a Cycloparaphenylene Template. ChemPhysChem, 2012, 13, 1479-1485.	2.1	26
178	Time-dependent quantum dynamical simulations of C₂condensation under extreme conditions. Physical Chemistry Chemical Physics, 2012, 14, 6273-6279.	2.8	14
179	Dynamics of Local Chirality during SWCNT Growth: Armchair versus Zigzag Nanotubes. Journal of the American Chemical Society, 2012, 134, 9311-9319.	13.7	38
180	Combined experimental and theoretical studies on the photophysical properties of cycloparaphenylenes. Organic and Biomolecular Chemistry, 2012, 10, 5979.	2.8	248

#	Article	IF	Citations
181	Simulation of Nuclear Dynamics of C60: From Vibrational Excitation by Near-IR Femtosecond Laser Pulses to Subsequent Nanosecond Rearrangement and Fragmentation. Progress in Theoretical Chemistry and Physics, 2012, , 149-177.	0.2	0
182	Thermal annealing of SiC nanoparticles induces SWNT nucleation: evidence for a catalyst-independent VSS mechanism. Physical Chemistry Chemical Physics, 2011, 13, 15673.	2.8	10
183	Regioselectivity control of graphene functionalization by ripples. Physical Chemistry Chemical Physics, 2011, 13, 19449.	2.8	46
184	SWNT Nucleation from Carbon-Coated SiO₂ Nanoparticles via a Vaporâ^'Solidâ^'Solid Mechanism. Journal of the American Chemical Society, 2011, 133, 621-628.	13.7	67
185	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.	13.7	95
186	Zwitterionic Ladder Stilbenes with Phosphonium and Borate Bridges: Intramolecular Cascade Cyclization and Structureâ€“Photophysical Properties Relationship. Organometallics, 2011, 30, 3870-3879.	2.3	63
187	Dramatic Reduction of IR Vibrational Cross Sections of Molecules Encapsulated in Carbon Nanotubes. Journal of the American Chemical Society, 2011, 133, 8191-8198.	13.7	36
188	Reactive Molecular Dynamics Simulation of Fullerene Combustion Synthesis: ReaxFF vs DFTB Potentials. Journal of Chemical Theory and Computation, 2011, 7, 2040-2048.	5.3	74
189	Growth of Linear Carbon Chains inside Thin Double-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2011, 115, 13166-13170.	3.1	81
190	A Ï€-stacked phenylacetylene dimer. Physical Chemistry Chemical Physics, 2011, 13, 16706.	2.8	33
191	Hot Giant Fullerenes Eject and Capture C₂ Molecules: QM/MD Simulations with Constant Density. Journal of Physical Chemistry C, 2011, 115, 22707-22716.	3.1	47
192	An n-Channel Two-Dimensional Covalent Organic Framework. Journal of the American Chemical Society, 2011, 133, 14510-14513.	13.7	330
193	Quantum Chemistry. , 2011, , 59-73.		5
194	Mechanisms of Single-Walled Carbon Nanotube Nucleation, Growth and Chirality-Control: Insights from QM/MD Simulations. , 2011, , .		0
195	A Simulation of Possible Carbon Nanotubes Slitting in a CMOS Compatible Way. Materials Express, 2011, 1, 343-349.	0.5	0
196	Dynamics Simulations of Fullerene and SWCNT Formation. , 2011, , 417-444.		0
197	Self-Consistent-Charge Density-Functional Tight-Binding/MD Simulation of Transition Metal Catalyst Particle Melting and Carbide Formation. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1755-1763.	0.4	13
198	Fullerenes: formation, stability, and reactivity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 350-367.	14.6	40

#	Article	IF	Citations
199	Electronic properties of hydrogenated quasiâ€freeâ€standing graphene. Physica Status Solidi (B): Basic Research, 2011, 248, 2639-2643.	1.5	17
200	Evidence for a New Twoâ€Dimensional C₄Hâ€Type Polymer Based on Hydrogenated Graphene. Advanced Materials, 2011, 23, 4497-4503.	21.0	90
201	Synthesis of 1â€Phosphaâ€2â€boraacenaphthenes: Reductive 1,2â€Aryl Migration of 1â€Diarylborylâ€8â€dichlorophosphinonaphthalenes. Angewandte Chemie - International Edition, 2011, 50, 10940-10943.	13.8	38
202	Do SiO2 and carbon-doped SiO2 nanoparticles melt? Insights from QM/MD simulations and ramifications regarding carbon nanotube growth. Chemical Physics Letters, 2011, 508, 235-241.	2.6	8
203	Determination of Local Chirality in Irregular Single-Walled Carbon Nanotubes Based on Individual Hexagons. Physical Review Letters, 2011, 107, 175505.	7.8	7
204	Relative Isomer Abundance of Fullerenes and Carbon Nanotubes Correlates with Kinetic Stability. Physical Review Letters, 2011, 107, 175506.	7.8	18
205	Carbon Spiral Helix: A Nanoarchitecture Derived from Monovacancy Defects in Graphene. Angewandte Chemie - International Edition, 2010, 49, 3200-3202.	13.8	17
206	Comparison of single-walled carbon nanotube growth from Fe and Ni nanoparticles using quantum chemical molecular dynamics methods. Carbon, 2010, 48, 3014-3026.	10.3	42
207	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.	10.3	19
208	Collision-induced fusion of twoC60fullerenes: Quantum chemical molecular dynamics simulations. Physical Review B, 2010, 82, .	3.2	30
209	Formation mechanism of polycyclic aromatic hydrocarbons in benzene combustion: Quantum chemical molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 224303.	3.0	25
210	Quantum Chemical Molecular Dynamics Simulations of Dynamic Fullerene Self-Assembly in Benzene Combustion. ACS Nano, 2010, 4, 583-583.	14.6	0
211	Quantum Chemical Prediction of Reaction Pathways and Rate Constants for Reactions of NO and NO₂ with Monovacancy Defects on Graphite (0001) Surfaces. Journal of Physical Chemistry C, 2010, 114, 8375-8382.	3.1	7
212	Atomic Structure and Energetic Stability of Complex Chiral Silicon Nanowires. Journal of Physical Chemistry C, 2010, 114, 14692-14696.	3.1	1
213	Polyyne Chain Growth and Ring Collapse Drives Ni-Catalyzed SWNT Growth: A QM/MD Investigation. Journal of Physical Chemistry C, 2010, 114, 8206-8211.	3.1	42
214	QM/MD Simulation of SWNT Nucleation on Transition-Metal Carbide Nanoparticles. Journal of the American Chemical Society, 2010, 132, 15699-15707.	13.7	93
215	Convergence in the Evolution of Nanodiamond Raman Spectra with Particle Size: A Theoretical Investigation. ACS Nano, 2010, 4, 4475-4486.	14.6	36
216	Mechanisms of Single-Walled Carbon Nanotube Nucleation, Growth, and Healing Determined Using QM/MD Methods. Accounts of Chemical Research, 2010, 43, 1375-1385.	15.6	117

#	Article	IF	Citations
217	Macro- and Microsimulations for a Sublimation Growth of SiC Single Crystals. Mathematical Problems in Engineering, 2009, 2009, 1-12.	1.1	1
218	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, .	3.2	30
219	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.	2.7	31
220	Milestones in molecular dynamics simulations of single-walled carbon nanotube formation: A brief critical review. Nano Research, 2009, 2, 755.	10.4	52
221	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.	2.0	20
222	Density-functional tight-binding molecular dynamics simulations of SWCNT growth by surface carbon diffusion on an iron cluster. Carbon, 2009, 47, 1270-1275.	10.3	44
223	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.	3.1	40
224	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.	3.1	27
225	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.	3.1	58
226	Quantum Chemical Molecular Dynamics Simulations of Dynamic Fullerene Self-Assembly in Benzene Combustion. ACS Nano, 2009, 3, 2241-2257.	14.6	46
227	Strong Electron Correlations Determine Energetic Stability and Electronic Properties of Er-Doped Goldberg-Type Silicon Quantum Dots. Journal of Physical Chemistry C, 2009, 113, 15964-15968.	3.1	3
228	Quantum Chemical Molecular Dynamics Simulation of Single-Walled Carbon Nanotube Cap Nucleation on an Iron Particle. ACS Nano, 2009, 3, 3413-3420.	14.6	96
229	RhI-catalyzed aldol-type reaction of organonitriles under mild conditions. Chemical Communications, 2008, , 2212.	4.1	62
230	Analysis of the Relationship between Reaction Energies of Electrophilic SWNT Additions and Sidewall Curvature: Chiral Nanotubes. Journal of Physical Chemistry C, 2008, 112, 12697-12705.	3.1	8
231	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.	14.6	98
232	Interaction of Acetone with Single Wall Carbon Nanotubes at Cryogenic Temperatures: A Combined Temperature Programmed Desorption and Theoretical Study. Langmuir, 2008, 24, 7848-7856.	3.5	30
233	THEORYâ€“EXPERIMENT RELATIONSHIP OF THE "SHRINKING HOT GIANT" ROAD OF DYNAMIC FULLERENE SELF-ASSEMBLY IN HOT CARBON VAPOR. Nano, 2007, 02, 21-30.	1.0	16
234	Quantum Chemical Molecular Dynamics Study of "Shrinking" of Hot Giant Fullerenes. Journal of Nanoscience and Nanotechnology, 2007, 7, 1662-1669.	0.9	36

#	Article	IF	Citations
235	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
236	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.	3.1	21
237	Mechanisms of the Reactions of W and W+ with NOx (x = 1, 2):â€‰ A Computational Study. Journal of Physical Chemistry A, 2007, 111, 982-991.	2.5	8
238	The Mechanisms of the Reactions of W and W+with COx(x= 1, 2):Â A Computational Studyâ€. Journal of Physical Chemistry A, 2007, 111, 6665-6673.	2.5	15
239	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.	3.1	77
240	Comparison of Interfacial Electron Transfer through Carboxylate and Phosphonate Anchoring Groupsâ€. Journal of Physical Chemistry A, 2007, 111, 6832-6842.	2.5	88
241	Comparison of Geometric, Electronic, and Vibrational Properties for Isomers of Small Fullerenes C20â"C36â€. Journal of Physical Chemistry A, 2007, 111, 6649-6657.	2.5	69
242	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.	13.7	37
243	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.	2.6	232
244	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.	3.0	21
245	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.	2.6	41
246	Mechanisms of the Reactions of W and W+with H2O:Â Computational Studies. Journal of Physical Chemistry A, 2006, 110, 4495-4501.	2.5	9
247	A Study of the Reaction of N+ with O2:â€‰ Experimental Quantification of NO+(a 3â^‘+) Production (298â^‘500 K) and Computational Study of the Overall Reaction Pathways. Journal of Physical Chemistry A, 2006, 110, 3080-3086.	2.5	5
248	Fe/C Interactions During SWNT Growth with C₂ Feedstock Molecules: A Quantum Chemical Molecular Dynamics Study. Journal of Nanoscience and Nanotechnology, 2006, 6, 1259-1270.	0.9	14
249	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.	3.0	40
250	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.	2.6	132
251	High-temperature quantum chemical molecular dynamics simulations of carbon nanostructure self-assembly processes. , 2005, , 875-889.		1
252	Towards formation of buckminsterfullerene C60 in quantum chemical molecular dynamics. Journal of Chemical Physics, 2005, 122, 014708.	3.0	43

#	Article	IF	Citations
253	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.	13.7	167
254	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.	2.5	52
255	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.	3.0	71
256	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
257	Oxidation of Alkyl Ions, CnH2n+1+(n= 1â˜5), in Reactions with O2and O3in the Gas Phase. Journal of Physical Chemistry A, 2004, 108, 1980-1989.	2.5	10
258	From C2Molecules to Self-Assembled Fullerenes in Quantum Chemical Molecular Dynamics. Nano Letters, 2003, 3, 1657-1664.	9.1	87
259	Formation of Fullerene Molecules from Carbon Nanotubes:Â A Quantum Chemical Molecular Dynamics Study. Nano Letters, 2003, 3, 465-470.	9.1	50
260	Ab initio theoretical studies of potential energy surfaces in the photodissociation of the vinyl radical. I. Ã*f* state dissociation. Journal of Chemical Physics, 2003, 119, 6524-6538.	3.0	9
261	The internal coordinate path Hamiltonian; application to methanol and malonaldehyde. Molecular Physics, 2003, 101, 3513-3525.	1.7	51
262	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.	2.5	34
263	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.	2.5	27
264	Ab initio investigation of the potential energy profiles for the gas phase CH4+O2+(2Îg) reaction system. Journal of Chemical Physics, 2001, 114, 6119-6127.	3.0	11
265	Dipole moments of highly vibrationally excited HCN: Theoretical prediction of an experimental diagnostic for delocalized states. Journal of Chemical Physics, 2001, 114, 7923-7934.	3.0	36
266	A molecular orbital study on H and H2 elimination pathways from methane, ethane, and propane. Journal of Chemical Physics, 2000, 113, 6139-6148.	3.0	17
267	Directab initiovariational calculation of vibrational energies of the H2Oâ‹¯Clâ˜ complex and resolution of experimental differences. Journal of Chemical Physics, 2000, 113, 8401-8403.	3.0	64
268	Prediction of the Post-Comatose Motor Function by Motor Evoked Potentials Obtained in the Acute Phase of Traumatic and Non-Traumatic Coma. Acta Neurochirurgica, 1999, 141, 841-848.	1.7	11
269	Ab initio and density functional study on the mechanism of the C2H2++methanol reaction. Journal of Chemical Physics, 1999, 111, 3978-3988.	3.0	7
270	Ab initio and density functional study on singlet and triplet states of artemisinin. Computational and Theoretical Chemistry, 1998, 454, 87-90.	1.5	12

#	Article	IF	Citations
271	Combined ab initio and density functional study on polaron to bipolaron transitions in oligophenyls and oligothiophenes. Journal of Chemical Physics, 1997, 107, 3021-3031.	3.0	52
272	Electronic Structure and Properties of Trihalogen Cations X3+and XY2+(X, Y = F, Cl, Br, I). Inorganic Chemistry, 1996, 35, 100-109.	4.0	16
273	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
274	Lithium- and chlorine-doped biphenyl dimers as models for interchain polarons and bipolarons â€" a density functional study. Chemical Physics Letters, 1996, 257, 592-600.	2.6	13
275	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.	3.0	45
276	Substituent Effects of -NO and -NO2, Groups in Aromatic Systems. Journal of Organic Chemistry, 1995, 60, 6744-6755.	3.2	49
277	Quantum Chemistry: Integrated Methods. , 0, , 3961-3974.		0