Stephan Irle

List of Publications by Year in Descending Order

276 papers	11,270 citations	57 h-index	95 g-index
305 ext. papers	12,965 ext. citations	6.9 avg, IF	6.32 L-index

#	Paper	IF	Citations
276	Dynamic aspects of graphene deformation and fracture from approximate density functional theory. *Carbon*, **2022**, 190, 183-193	10.4	1
275	Design of tough adhesive from commodity thermoplastics through dynamic crosslinking. *Science Advances*, **2021**, 7, eabk2451	14.3	10
274	How the Size and Density of Charge-Transfer Excitons Depend on Heterojunctions Architecture. *Journal of Physical Chemistry C*, **2021**, 125, 5458-5474	3.8	3
273	Strain-Induced Growth of Twisted Bilayers during the Coalescence of Monolayer MoS Crystals. *ACS Nano*, **2021**, 15, 4504-4517	16.7	5
272	Density-Functional Tight-Binding Parameters for Bulk Zirconium: A Case Study for Repulsive Potentials. *Journal of Physical Chemistry A*, **2021**, 125, 2184-2196	2.8	1
271	Hydroxide Anion Transport in Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2021**, 143, 8970-8975	16.4	15
270	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	3.9	1
269	Density Functional Tight-Binding Simulations Reveal the Presence of Surface Defects on the Quartz (101) Water Interface. *Journal of Physical Chemistry C*, **2021**, 125, 16246-16255	3.8	
268	The FMO-DFTB Method **2021**, 459-485		1
267	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	4.2	1
266	Methane Adsorption on Heteroatom-Modified of Porous Carbon Surfaces. *Journal of Physical Chemistry A*, **2021**, 125, 6042-6058	2.8	0
265	Investigating the Accuracy of Water Models through the Van Hove Correlation Function. *Journal of Chemical Theory and Computation*, **2021**, 17, 5992-6005	6.4	3
264	Pre-Sodiated TiCT MXene Structure and Behavior as Electrode for Sodium-Ion Capacitors. *ACS Nano* , **2021**, 15, 2994-3003	16.7	21
263	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. *Journal of Chemical Information and Modeling*, **2020**, 60, 5832-5852	6.1	71
262	Boosting electrosynthesis of ammonia on surface-engineered MXene Ti3C2. *Nano Energy*, **2020**, 72, 104681	16.1	48
261	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *Journal of Chemical Physics*, **2020**, 152, 124101	3.9	210
260	Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst. *Journal of the American Chemical Society*, **2020**, 142, 7655-7667	16.4	33

259	Topology-Templated Synthesis of Crystalline Porous Covalent Organic Frameworks. *Angewandte Chemie - International Edition*, **2020**, 59, 12162-12169	16.4	34
258	Topology-Templated Synthesis of Crystalline Porous Covalent Organic Frameworks. *Angewandte Chemie*, **2020**, 132, 12260-12267	3.6	10
257	Protein Molecular Dynamics Simulations with Approximate QM: What Can We Learn?. *Methods in Molecular Biology*, **2020**, 2114, 149-161	1.4	
256	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. *ChemRxiv*, **2020**,	4.4	7
255	Density-functional tight-binding for phosphine-stabilized nanoscale gold clusters. *Chemical Science*, **2020**, 11, 13113-13128	9.4	13
254	Recent developments in the general atomic and molecular electronic structure system. *Journal of Chemical Physics*, **2020**, 152, 154102	3.9	274
253	The helix-inversion mechanism in double-stranded helical oligomers bridged by rotary cyclic boronate esters. *Journal of Computational Chemistry*, **2019**, 40, 2036-2042	3.5	
252	The Fragment Molecular Orbital Method Based on Long-Range Corrected Density-Functional Tight-Binding. *Journal of Chemical Theory and Computation*, **2019**, 15, 3008-3020	6.4	27
251	Phenyleneethynylene trimer-based rigid-flexible [2+2] macrocycles for nucleic acid labelling in live cells. *Chemical Communications*, **2019**, 55, 5930-5933	5.8	11
250	Structural transformations of graphene exposed to nitrogen plasma: quantum chemical molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2019**, 21, 12112-12120	3.6	5
249	Water-mediated deracemization of a bisporphyrin helicate assisted by diastereoselective encapsulation of chiral guests. *Nature Communications*, **2019**, 10, 1457	17.4	15
248	Artificial neural network correction for density-functional tight-binding molecular dynamics simulations. *MRS Communications*, **2019**, 9, 867-873	2.7	20
247	How does acetonitrile modulate single-walled carbon nanotube diameter during CVD growth?. *Carbon*, **2019**, 146, 535-541	10.4	7
246	Nonadiabatic excited-state intramolecular proton transfer in 3-hydroxyflavone: S state involvement via multi-mode effect. *Journal of Chemical Physics*, **2019**, 151, 214304	3.9	7
245	Density-Functional Tight-Binding for Platinum Clusters and Bulk: Electronic vs Repulsive Parameters. *MRS Advances*, **2019**, 4, 1821-1832	0.7	1
244	Chiral-selective etching effects on carbon nanotube growth at edge carbon atoms. *Journal of Computational Chemistry*, **2019**, 40, 375-380	3.5	4
243	Low-energy hydrogen uptake by small-cage Cn and Cn-1B fullerenes. *Carbon*, **2018**, 134, 189-198	10.4	11
242	Keiji Morokuma (1934-2017). *Angewandte Chemie - International Edition*, **2018**, 57, 2288-2289	16.4	

241	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	9.4	36
240	Parametrization and Benchmark of Long-Range Corrected DFTB2 for Organic Molecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 115-125	6.4	41
239	A New Porous Polymer for Highly Efficient Capacitive Energy Storage. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 202-209	8.3	54
238	Simulations of the synthesis of boron-nitride nanostructures in a hot, high pressure gas volume. *Chemical Science*, **2018**, 9, 3803-3819	9.4	23
237	Implementation of replica-exchange umbrella sampling in GAMESS. *Computer Physics Communications*, **2018**, 228, 152-162	4.2	7
236	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	3.9	1
235	Decoding Oxyanion Aqueous Solvation Structure: A Potassium Nitrate Example at Saturation. *Journal of Physical Chemistry B*, **2018**, 122, 7584-7589	3.4	13
234	Focus-Induced Photoresponse: a novel way to measure distances with photodetectors. *Scientific Reports*, **2018**, 8, 9208	4.9	10
233	Inducing regioselective chemical reactivity in graphene with alkali metal intercalation. *Physical Chemistry Chemical Physics*, **2018**, 20, 19987-19994	3.6	3
232	Conformational dynamics of human protein kinase CK2 and its effect on function and inhibition. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 344-353	4.2	8
231	. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 1610-1619	8.3	33
230	Statistical Mechanics-Based Theoretical Investigation of Solvation Effects on Glucose Anomer Preferences. *Journal of Physical Chemistry B*, **2018**, 122, 290-296	3.4	4
229	A femtomolar-range suicide germination stimulant for the parasitic plant. *Science*, **2018**, 362, 1301-1305	33.3	59
228	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	3.9	5
227	When finite becomes infinite: convergence properties of vibrational spectra of oligomer chains. *Journal of Molecular Modeling*, **2018**, 24, 288	2	4
226	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	16.4	126
225	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	2.8	5
224	Theoretical analysis of orientations and tautomerization of genistein in cyclodextrin. *Journal of Molecular Liquids*, **2018**, 265, 16-23	6	5

223	A New Triazine-Based Covalent Organic Framework for High-Performance Capacitive Energy Storage. *ChemSusChem*, **2017**, 10, 921-929	8.3	88
222	Theoretical Studies on Ethanol Dissociation on Iron Nanoparticles in the Early Stage of SWCNT Growth. *Journal of Physical Chemistry C*, **2017**, 121, 2276-2284	3.8	13
221	Förster Resonance Energy Transfer between Fluorescent Proteins: Efficient Transition Charge-Based Study. *Journal of Physical Chemistry C*, **2017**, 121, 4220-4238	3.8	8
220	Cryptic bioactivity capacitated by synthetic hybrid plant peptides. *Nature Communications*, **2017**, 8, 14318	17.4	20
219	Theoretical rationalization for reduced charge recombination in bulky carbazole-based sensitizers in solar cells. *Journal of Computational Chemistry*, **2017**, 38, 901-909	3.5	2
218	Double-Stranded Helical Oligomers Covalently Bridged by Rotary Cyclic Boronate Esters. *Chemistry - an Asian Journal*, **2017**, 12, 927-935	4.5	12
217	Theoretical Elucidation of Potential Enantioselectivity in a Pd-Catalyzed Aromatic C-H Coupling Reaction. *Journal of Organic Chemistry*, **2017**, 82, 4900-4906	4.2	12
216	QM/MD Simulations on Graphene Hydrogenation/Deuteration: CxH/D Formation Mechanism and Isotope Effect. *Journal of Physical Chemistry C*, **2017**, 121, 8480-8489	3.8	2
215	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	3.8	2
214	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	3.8	6
213	Importance of oxygen in single-walled carbon nanotube growth: Insights from QM/MD simulations. *Carbon*, **2017**, 121, 292-300	10.4	9
212	Electrically Activated Conductivity and White Light Emission of a Hydrocarbon Nanoring□Iodine Assembly. *Angewandte Chemie*, **2017**, 129, 11348-11354	3.6	16
211	Er Photoluminescence in Er@C and ErC@C Metallofullerenes Elucidated by Density Functional Theory. *Inorganic Chemistry*, **2017**, 56, 6576-6583	5.1	6
210	Quantum chemical molecular dynamics simulation of carbon nanotube□graphene fusion. *Molecular Simulation*, **2017**, 43, 1269-1276	2	5
209	Constructing Sulfonic Acid Functionalized Anthracene Derived Conjugated Porous Organic Polymer for Efficient Metal-Free Catalytic Acetalization of Bio-Glycerol. *ChemistrySelect*, **2017**, 2, 4705-4716	1.8	12
208	Polymorphism of [6]Cycloparaphenylene for Packing Structure-dependent Host□Guest Interaction. *Chemistry Letters*, **2017**, 46, 855-857	1.7	19
207	Structural influence of transition metal (Sc, Y, and Lu) atoms inside gold nanoparticles. *International Journal of Quantum Chemistry*, **2017**, 117, e25371	2.1	3
206	Indirect Intersystem Crossing (S -iT/T -iT) Promoted by the Jahn-Teller Effect in Cycloparaphenylenes. *Journal of Chemical Theory and Computation*, **2017**, 13, 4944-4949	6.4	5

205	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	3.8	12
204	Unraveling the plasma-material interface with real time diagnosis of dynamic boron conditioning in extreme tokamak plasmas. *Nuclear Fusion*, **2017**, 57, 086050	3.3	7
203	Development of density-functional tight-binding repulsive potentials for bulk zirconia using particle swarm optimization algorithm **2017**,		2
202	Quantum chemical prediction of vibrational spectra of large molecular systems with radical or metallic electronic structure. *Chemical Physics Letters*, **2017**, 667, 317-321	2.5	7
201	Electrically Activated Conductivity and White Light Emission of a Hydrocarbon Nanoring-Iodine Assembly. *Angewandte Chemie - International Edition*, **2017**, 56, 11196-11202	16.4	49
200	Chiral-Selective Carbon Nanotube Etching with Ammonia: A Quantum Chemical Investigation. *Journal of Physical Chemistry C*, **2016**, 120, 19862-19870	3.8	7
199	Light-melt adhesive based on dynamic carbon frameworks in a columnar liquid-crystal phase. *Nature Communications*, **2016**, 7, 12094	17.4	79
198	Two-dimensional artificial light-harvesting antennae with predesigned high-order structure and robust photosensitising activity. *Scientific Reports*, **2016**, 6, 32944	4.9	29
197	Spanning the Parameter Space of Chemical Vapor Deposition Graphene Growth with Quantum Chemical Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 13851-13864	3.8	12
196	QM/MD studies on graphene growth from small islands on the Ni(111) surface. *Nanoscale*, **2016**, 8, 3067-74	7.7	17
195	Self-assembly of endohedral metallofullerenes: a decisive role of cooling gas and metal-carbon bonding. *Nanoscale*, **2016**, 8, 3796-808	7.7	20
194	Self-Consistent Optimization of Excited States within Density-Functional Tight-Binding. *Journal of Chemical Theory and Computation*, **2016**, 12, 313-23	6.4	8
193	Automatized Parameterization of DFTB Using Particle Swarm Optimization. *Journal of Chemical Theory and Computation*, **2016**, 12, 53-64	6.4	41
192	Automatized Parameterization of the Density-functional Tight-binding Method. II. Two-center Integrals. *Journal of the Chinese Chemical Society*, **2016**, 63, 57-68	1.5	11
191	Diversity in electronic structure and vibrational properties of fullerene isomers correlates with cage curvature. *Carbon*, **2016**, 100, 484-491	10.4	8
190	Cycloparaphenylene as a molecular porous carbon solid with uniform pores exhibiting adsorption-induced softness. *Chemical Science*, **2016**, 7, 4204-4210	9.4	44
189	Ab initio and first principles theoretical investigations of triplet–triplet fluorescence in trimethylenemethane biradicals. *RSC Advances*, **2016**, 6, 83668-83672	3.7	2
188	Three pillars for achieving quantum mechanical molecular dynamics simulations of huge systems: Divide-and-conquer, density-functional tight-binding, and massively parallel computation. *Journal of Computational Chemistry*, **2016**, 37, 1983-92	3.5	72

187	Glucose transformation to 5-hydroxymethylfurfural in acidic ionic liquid: A quantum mechanical study. *Journal of Computational Chemistry*, **2016**, 37, 327-35	3.5	19
186	A Macrocyclic Fluorophore Dimer with Flexible Linkers: Bright Excimer Emission with a Long Fluorescence Lifetime. *Angewandte Chemie - International Edition*, **2016**, 55, 7131-5	16.4	34
185	A Macrocyclic Fluorophore Dimer with Flexible Linkers: Bright Excimer Emission with a Long Fluorescence Lifetime. *Angewandte Chemie*, **2016**, 128, 7247-7251	3.6	15
184	A global reaction route mapping-based kinetic Monte Carlo algorithm. *Journal of Chemical Physics*, **2016**, 145, 024105	3.9	11
183	Theoretical Investigation of Molecular and Electronic Structures of Buckminsterfullerene-Silicon Quantum Dot Systems. *Journal of Physical Chemistry A*, **2016**, 120, 9767-9775	2.8	2
182	Stacked antiaromatic porphyrins. *Nature Communications*, **2016**, 7, 13620	17.4	76
181	Molecular dynamical modelling of endohedral fullerenes formation in plasma. *IOP Conference Series: Materials Science and Engineering*, **2016**, 110, 012078	0.4	
180	Implementation of replica-exchange umbrella sampling in the DFTB+ semiempirical quantum chemistry package. *Computer Physics Communications*, **2016**, 204, 1-10	4.2	5
179	Understanding of the Off-On Response Mechanism in Caged Fluorophores Based on Quantum and Statistical Mechanics. *Journal of Physical Chemistry B*, **2016**, 120, 4449-56	3.4	6
178	Theoretical analysis of structural diversity of covalent organic framework: Stacking isomer structures thermodynamics and kinetics. *Chemical Physics Letters*, **2016**, 664, 101-107	2.5	10
177	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, 3241-7	16.4	238
176	Quantum Chemical Simulation of Carbon Nanotube Nucleation on Al2O3 Catalysts via CH4 Chemical Vapor Deposition. *Journal of the American Chemical Society*, **2015**, 137, 9281-8	16.4	24
175	Rational design of crystalline supermicroporous covalent organic frameworks with triangular topologies. *Nature Communications*, **2015**, 6, 7786	17.4	185
174	Fabrication and optical probing of highly extended, ultrathin graphene nanoribbons in carbon nanotubes. *ACS Nano*, **2015**, 9, 5034-40	16.7	29
173	C?H Activation Generates Period-Shortening Molecules That Target Cryptochrome in the Mammalian Circadian Clock. *Angewandte Chemie*, **2015**, 127, 7299-7303	3.6	2
172	C-H activation generates period-shortening molecules that target cryptochrome in the mammalian circadian clock. *Angewandte Chemie - International Edition*, **2015**, 54, 7193-7	16.4	50
171	Insights into carbon nanotube and graphene formation mechanisms from molecular simulations: a review. *Reports on Progress in Physics*, **2015**, 78, 036501	14.4	80
170	Third-order density-functional tight-binding combined with the fragment molecular orbital method. *Chemical Physics Letters*, **2015**, 636, 90-96	2.5	28

169	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, 5034-9	6.4	39
168	Nearly exclusive growth of small diameter semiconducting single-wall carbon nanotubes from organic chemistry synthetic end-cap molecules. *Nano Letters*, **2015**, 15, 586-95	11.5	69
167	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	2.9	2
166	Understanding the On-Off Switching Mechanism in Cationic Tetravalent Group-V-Based Fluoride Molecular Sensors Using Orbital Analysis. *Journal of Physical Chemistry A*, **2015**, 119, 12693-8	2.8	9
165	R□ □ktitelbild: C?H Activation Generates Period-Shortening Molecules That Target Cryptochrome in the Mammalian Circadian Clock (Angew. Chem. 24/2015). *Angewandte Chemie*, **2015**, 127, 7306-7306	3.6	
164	Designed synthesis of double-stage two-dimensional covalent organic frameworks. *Scientific Reports*, **2015**, 5, 14650	4.9	81
163	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	5.1	10
162	Creation of Superheterojunction Polymers via Direct Polycondensation: Segregated and Bicontinuous Donor-Acceptor □Columnar Arrays in Covalent Organic Frameworks for Long-Lived Charge Separation. *Journal of the American Chemical Society*, **2015**, 137, 7817-27	16.4	152
161	Development of Small-Molecule Cryptochrome Stabilizer Derivatives as Modulators of the Circadian Clock. *ChemMedChem*, **2015**, 10, 1489-97	3.7	33
160	Hybridization of a flexible cyclooctatetraene core and rigid aceneimide wings for multiluminescent flapping □ystems. *Chemistry - A European Journal*, **2014**, 20, 2193-200	4.8	68
159	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	3.8	24
158	Constraint-induced structural deformation of planarized triphenylboranes in the excited state. *Chemical Science*, **2014**, 5, 1296-1304	9.4	46
157	Step-edge self-assembly during graphene nucleation on a nickel surface: QM/MD simulations. *Nanoscale*, **2014**, 6, 140-4	7.7	22
156	Density-Functional Tight-Binding Combined with the Fragment Molecular Orbital Method. *Journal of Chemical Theory and Computation*, **2014**, 10, 4801-12	6.4	67
155	Catalytic covalent organic frameworks via pore surface engineering. *Chemical Communications*, **2014**, 50, 1292-4	5.8	243
154	Molecular simulation of water and hydration effects in different environments: challenges and developments for DFTB based models. *Journal of Physical Chemistry B*, **2014**, 118, 11007-27	3.4	74
153	Quantum Dynamics Simulations Reveal Vibronic Effects on the Optical Properties of [n]Cycloparaphenylenes. *Journal of Chemical Theory and Computation*, **2014**, 10, 4025-36	6.4	25
152	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. *Chemical Science*, **2014**, 5, 3493-3500	9.4	36

151	A strap strategy for construction of an excited-state intramolecular proton transfer (ESIPT) system with dual fluorescence. *Angewandte Chemie - International Edition*, **2014**, 53, 8231-5	16.4	88
150	Direct evidence of active and inactive phases of Fe catalyst nanoparticles for carbon nanotube formation. *Journal of Catalysis*, **2014**, 319, 54-60	7.3	47
149	Theoretical study of cellobiose hydrolysis to glucose in ionic liquids. *Chemical Physics Letters*, **2014**, 603, 7-12	2.5	23
148	Two-dimensional tetrathiafulvalene covalent organic frameworks: towards latticed conductive organic salts. *Chemistry - A European Journal*, **2014**, 20, 14608-13	4.8	109
147	A Strap Strategy for Construction of an Excited-State Intramolecular Proton Transfer (ESIPT) System with Dual Fluorescence. *Angewandte Chemie*, **2014**, 126, 8370-8374	3.6	23
146	Super-reduced polyoxometalates: excellent molecular cluster battery components and semipermeable molecular capacitors. *Journal of the American Chemical Society*, **2014**, 136, 9042-52	16.4	136
145	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	2	4
144	Theoretical investigation of molecular and electronic structure changes of the molecular magnet Mn12 cluster upon super-reduction. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 517-521	2.5	3
143	Critical interpretation of CH- and OH- stretching regions for infrared spectra of methanol clusters (CH□OH)n (n = 2-5) using self-consistent-charge density functional tight-binding molecular dynamics simulations. *Journal of Chemical Physics*, **2014**, 141, 094303	3.9	17
142	Growth mechanisms and selectivity for graphene or carbon nanotube formation on SiC (0001□): A density-functional tight-binding molecular dynamics study. *Chemical Physics Letters*, **2014**, 595-596, 266-271	2.5	8
141	Nonequilibrium quantum chemical molecular dynamics simulations of C60 to SiC heterofullerene conversion. *Carbon*, **2014**, 68, 285-295	10.4	12
140	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	2.5	17
139	Quantum chemical simulations reveal acetylene-based growth mechanisms in the chemical vapor deposition synthesis of carbon nanotubes. *Carbon*, **2014**, 72, 22-37	10.4	44
138	Stochastic structure determination for conformationally flexible heterogenous molecular clusters: application to ionic liquids. *Journal of Computational Chemistry*, **2013**, 34, 2591-600	3.5	33
137	Photochemical double 5-exo cyclization of alkenyl-substituted dithienylacetylenes: efficient synthesis of diarylated dithienofulvalenes. *Angewandte Chemie - International Edition*, **2013**, 52, 10519-23	16.4	10
136	Temperature Dependence of Catalyst-Free Chirality-Controlled Single-Walled Carbon Nanotube Growth from Organic Templates. *Journal of Physical Chemistry Letters*, **2013**, 4, 3176-3180	6.4	10
135	Conjugated organic framework with three-dimensionally ordered stable structure and delocalized □clouds. *Nature Communications*, **2013**, 4, 2736	17.4	404
134	Atom-by-atom simulations of graphene growth by decomposition of SiC (0001): Impact of the substrate steps. *Applied Physics Letters*, **2013**, 103, 141602	3.4	21

133	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	6.4	15
132	Carbon Coating Precedes SWCNT Nucleation on Silicon Nanoparticles: Insights from QM/MD Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 4238-4244	3.8	11
131	Large pore donor–acceptor covalent organic frameworks. *Chemical Science*, **2013**, 4, 4505	9.4	100
130	Control of crystallinity and porosity of covalent organic frameworks by managing interlayer interactions based on self-complementary electronic force. *Journal of the American Chemical Society*, **2013**, 135, 546-9	16.4	189
129	Electrical switching behavior of a [60]fullerene-based molecular wire encapsulated in a syndiotactic poly(methyl methacrylate) helical cavity. *Angewandte Chemie - International Edition*, **2013**, 52, 1049-53	16.4	46
128	Electrical Switching Behavior of a [60]Fullerene-Based Molecular Wire Encapsulated in a Syndiotactic Poly(methyl methacrylate) Helical Cavity. *Angewandte Chemie*, **2013**, 125, 1083-1087	3.6	10
127	Innentitelbild: Electrical Switching Behavior of a [60]Fullerene-Based Molecular Wire Encapsulated in a Syndiotactic Poly(methyl methacrylate) Helical Cavity (Angew. Chem. 3/2013). *Angewandte Chemie*, **2013**, 125, 804-804	3.6	
126	Quantum chemical investigation of epoxide and ether groups in graphene oxide and their vibrational spectra. *Physical Chemistry Chemical Physics*, **2013**, 15, 3725-35	3.6	39
125	Origin of the size-dependent fluorescence blueshift in [n]cycloparaphenylenes. *Chemical Science*, **2013**, 4, 187-195	9.4	66
124	High-temperature transformation of Fe-decorated single-wall carbon nanohorns to nanooysters: a combined experimental and theoretical study. *Nanoscale*, **2013**, 5, 1849-57	7.7	10
123	Charge dynamics in a donor-acceptor covalent organic framework with periodically ordered bicontinuous heterojunctions. *Angewandte Chemie - International Edition*, **2013**, 52, 2017-21	16.4	217
122	TICT fluorescence of N-borylated 2,5-diarylpyrroles: a gear like dual motion in the excited state. *Dalton Transactions*, **2013**, 42, 620-4	4.3	55
121	Nucleation of Graphene Precursors on Transition Metal Surfaces: Insights from Theoretical Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 14858-14864	3.8	38
120	A conjugated system with flexibility and rigidity that shows environment-dependent RGB luminescence. *Journal of the American Chemical Society*, **2013**, 135, 8842-5	16.4	146
119	Kinetic Isotope Effect in the Hydrogenation and Deuteration of Graphene. *Advanced Functional Materials*, **2013**, 23, 1628-1635	15.6	32
118	Growth of carbon nanotubes via twisted graphene nanoribbons. *Nature Communications*, **2013**, 4, 2548	17.4	77
117	Stochastic Search of Molecular Cluster Interaction Energy Surfaces with Coupled Cluster Quality Prediction. The Phenylacetylene Dimer. *Journal of Chemical Theory and Computation*, **2013**, 9, 3848-54	6.4	2
116	Charge Dynamics in A Donor–Acceptor Covalent Organic Framework with Periodically Ordered Bicontinuous Heterojunctions. *Angewandte Chemie*, **2013**, 125, 2071-2075	3.6	46

115	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, 4918-24	16.4	289
114	Sub-surface nucleation of graphene precursors near a Ni(111) step-edge. *Chemical Communications*, **2012**, 48, 7937-9	5.8	37
113	Optimization of a Genetic Algorithm for the Functionalization of Fullerenes. *Journal of Chemical Theory and Computation*, **2012**, 8, 1841-51	6.4	13
112	Substituent effects on twisted internal charge transfer excited states of N-borylated carbazoles and (diphenylamino)boranes. *Journal of Physical Chemistry A*, **2012**, 116, 1151-8	2.8	31
111	Theoretical Investigation of the Structures and Dynamics of Crystalline Molecular Gyroscopes. *Journal of Physical Chemistry C*, **2012**, 116, 24845-24854	3.8	23
110	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, 15887-96	16.4	48
109	Effects of Molecular Dynamics Thermostats on Descriptions of Chemical Nonequilibrium. *Journal of Chemical Theory and Computation*, **2012**, 8, 4019-28	6.4	11
108	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, 7154-60	2.8	46
107	Modeling Charge Transfer in Fullerene Collisions via Real-Time Electron Dynamics. *Journal of Physical Chemistry Letters*, **2012**, 3, 1536-42	6.4	20
106	Delocalization errors in a hubbard-like model: Consequences for density-functional tight-binding calculations of molecular systems. *International Journal of Quantum Chemistry*, **2012**, 112, 1701-1711	2.1	19
105	Molecular and electronic structures of endohedral fullerenes, Sc2C2@C3v(8)-82 and Sc2@C3v(8)-82: Benchmark for SCC-DFTB and proposal of new inner cluster structures. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 324-334	1.3	15
104	High-rate charge-carrier transport in porphyrin covalent organic frameworks: switching from hole to electron to ambipolar conduction. *Angewandte Chemie - International Edition*, **2012**, 51, 2618-22	16.4	291
103	Dimerization-Initiated Preferential Formation of Coronene-Based Graphene Nanoribbons in Carbon Nanotubes. *Journal of Physical Chemistry C*, **2012**, 116, 15141-15145	3.8	74
102	An ambipolar conducting covalent organic framework with self-sorted and periodic electron donor-acceptor ordering. *Advanced Materials*, **2012**, 24, 3026-31	24	217
101	High-Rate Charge-Carrier Transport in Porphyrin Covalent Organic Frameworks: Switching from Hole to Electron to Ambipolar Conduction. *Angewandte Chemie*, **2012**, 124, 2672-2676	3.6	86
100	Theoretical insights into chirality-controlled SWCNT growth from a cycloparaphenylene template. *ChemPhysChem*, **2012**, 13, 1479-85	3.2	26
99	Time-dependent quantum dynamical simulations of C2 condensation under extreme conditions. *Physical Chemistry Chemical Physics*, **2012**, 14, 6273-9	3.6	12
98	Dynamics of local chirality during SWCNT growth: armchair versus zigzag nanotubes. *Journal of the American Chemical Society*, **2012**, 134, 9311-9	16.4	36

97	Combined experimental and theoretical studies on the photophysical properties of cycloparaphenylenes. *Organic and Biomolecular Chemistry*, **2012**, 10, 5979-84	3.9	202
96	Atomistic Mechanism of Carbon Nanostructure Self-Assembly as Predicted by Nonequilibrium QM/MD Simulations **2012**, 103-172		4
95	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	0.6	
94	QM/MD Simulations of High-Temperature SWCNT Self-capping **2012**, 53-68		
93	A Ⅱstacked phenylacetylene dimer. *Physical Chemistry Chemical Physics*, **2011**, 13, 16706-12	3.6	31
92	Hot Giant Fullerenes Eject and Capture C2 Molecules: QM/MD Simulations with Constant Density. *Journal of Physical Chemistry C*, **2011**, 115, 22707-22716	3.8	42
91	An n-channel two-dimensional covalent organic framework. *Journal of the American Chemical Society*, **2011**, 133, 14510-3	16.4	277
90	Quantum Chemistry: Propagation of Electronic Structure on a GPU **2011**, 59-73		5
89	Dynamics Simulations of Fullerene and SWCNT Formation **2011**, 417-444		
88	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	0.3	10
87	Fullerenes: formation, stability, and reactivity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 350-367	7.9	36
86	Electronic properties of hydrogenated quasi-free-standing graphene. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 2639-2643	1.3	15
85	Evidence for a new two-dimensional C4H-type polymer based on hydrogenated graphene. *Advanced Materials*, **2011**, 23, 4497-503	24	86
84	Synthesis of 1-phospha-2-boraacenaphthenes: reductive 1,2-aryl migration of 1-diarylboryl-8-dichlorophosphinonaphthalenes. *Angewandte Chemie - International Edition*, **2011**, 50, 10940-3	16.4	32
83	Thermal annealing of SiC nanoparticles induces SWNT nucleation: evidence for a catalyst-independent VSS mechanism. *Physical Chemistry Chemical Physics*, **2011**, 13, 15673-80	3.6	10
82	Regioselectivity control of graphene functionalization by ripples. *Physical Chemistry Chemical Physics*, **2011**, 13, 19449-53	3.6	39
81	SWNT nucleation from carbon-coated SiO2 nanoparticles via a vapor-solid-solid mechanism. *Journal of the American Chemical Society*, **2011**, 133, 621-8	16.4	61
80	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, 18837-42	16.4	82

79	Zwitterionic Ladder Stilbenes with Phosphonium and Borate Bridges: Intramolecular Cascade Cyclization and Structure–Photophysical Properties Relationship. *Organometallics*, **2011**, 30, 3870-3879	3.8	58
78	Dramatic reduction of IR vibrational cross sections of molecules encapsulated in carbon nanotubes. *Journal of the American Chemical Society*, **2011**, 133, 8191-8	16.4	33
77	Reactive Molecular Dynamics Simulation of Fullerene Combustion Synthesis: ReaxFF vs DFTB Potentials. *Journal of Chemical Theory and Computation*, **2011**, 7, 2040-8	6.4	61
76	Growth of Linear Carbon Chains inside Thin Double-Wall Carbon Nanotubes. *Journal of Physical Chemistry C*, **2011**, 115, 13166-13170	3.8	67
75	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	2.5	7
74	Determination of local chirality in irregular single-walled carbon nanotubes based on individual hexagons. *Physical Review Letters*, **2011**, 107, 175505	7.4	7
73	Relative isomer abundance of fullerenes and carbon nanotubes correlates with kinetic stability. *Physical Review Letters*, **2011**, 107, 175506	7.4	18
72	Collision-induced fusion of two C60 fullerenes: Quantum chemical molecular dynamics simulations. *Physical Review B*, **2010**, 82,	3.3	26
71	Formation mechanism of polycyclic aromatic hydrocarbons in benzene combustion: Quantum chemical molecular dynamics simulations. *Journal of Chemical Physics*, **2010**, 132, 224303	3.9	24
70	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	3.8	7
69	Atomic Structure and Energetic Stability of Complex Chiral Silicon Nanowires. *Journal of Physical Chemistry C*, **2010**, 114, 14692-14696	3.8	1
68	Polyyne Chain Growth and Ring Collapse Drives Ni-Catalyzed SWNT Growth: A QM/MD Investigation. *Journal of Physical Chemistry C*, **2010**, 114, 8206-8211	3.8	42
67	QM/MD simulation of SWNT nucleation on transition-metal carbide nanoparticles. *Journal of the American Chemical Society*, **2010**, 132, 15699-707	16.4	86
66	Convergence in the evolution of nanodiamond Raman spectra with particle size: a theoretical investigation. *ACS Nano*, **2010**, 4, 4475-86	16.7	33
65	Mechanisms of single-walled carbon nanotube nucleation, growth, and healing determined using QM/MD methods. *Accounts of Chemical Research*, **2010**, 43, 1375-85	24.3	103
64	Carbon spiral helix: a nanoarchitecture derived from monovacancy defects in graphene. *Angewandte Chemie - International Edition*, **2010**, 49, 3200-2	16.4	16
63	Comparison of single-walled carbon nanotube growth from Fe and Ni nanoparticles using quantum chemical molecular dynamics methods. *Carbon*, **2010**, 48, 3014-3026	10.4	40
62	Temperature and pressure dependence of molecular adsorption on single wall carbon nanotubes and the existence of an adsorption/desorption pressure gap. *Carbon*, **2010**, 48, 1867-1875	10.4	16

61	Macro- and Microsimulations for a Sublimation Growth of SiC Single Crystals. *Mathematical Problems in Engineering*, **2009**, 2009, 1-12	1.1	1
60	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,	3.3	30
59	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	3.3	28
58	Milestones in molecular dynamics simulations of single-walled carbon nanotube formation: A brief critical review. *Nano Research*, **2009**, 2, 755-767	10	45
57	Comparison of geometric, electronic, and vibrational properties for all pentagon/hexagon-bearing isomers of fullerenes C38, C40, and C42. *International Journal of Quantum Chemistry*, **2009**, 109, 1999-2011	2.1	18
56	Density-functional tight-binding molecular dynamics simulations of SWCNT growth by surface carbon diffusion on an iron cluster. *Carbon*, **2009**, 47, 1270-1275	10.4	40
55	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	3.8	40
54	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	3.8	25
53	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	3.8	57
52	Quantum chemical molecular dynamics simulations of dynamic fullerene self-assembly in benzene combustion. *ACS Nano*, **2009**, 3, 2241-57	16.7	44
51	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	3.8	2
50	Quantum chemical molecular dynamics simulation of single-walled carbon nanotube cap nucleation on an iron particle. *ACS Nano*, **2009**, 3, 3413-20	16.7	85
49	RhI-catalyzed aldol-type reaction of organonitriles under mild conditions. *Chemical Communications* , **2008**, 2212-4	5.8	58
48	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	3.8	7
47	Rapid growth of a single-walled carbon nanotube on an iron cluster: density-functional tight-binding molecular dynamics simulations. *ACS Nano*, **2008**, 2, 1437-44	16.7	94
46	Interaction of acetone with single wall carbon nanotubes at cryogenic temperatures: a combined temperature programmed desorption and theoretical study. *Langmuir*, **2008**, 24, 7848-56	4	26
45	Mechanisms of the reactions of W and W+ with NOx (x=1, 2): a computational study. *Journal of Physical Chemistry A*, **2007**, 111, 982-91	2.8	5
44	The mechanisms of the reactions of W and W+ with COx (x=1, 2): a computational study. *Journal of Physical Chemistry A*, **2007**, 111, 6665-73	2.8	13

43	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	3.8	72
42	Comparison of interfacial electron transfer through carboxylate and phosphonate anchoring groups. *Journal of Physical Chemistry A*, **2007**, 111, 6832-42	2.8	84
41	Comparison of geometric, electronic, and vibrational properties for isomers of small fullerenes C20-C36. *Journal of Physical Chemistry A*, **2007**, 111, 6649-57	2.8	60
40	THEORY–EXPERIMENT RELATIONSHIP OF THE "SHRINKING HOT GIANT" ROAD OF DYNAMIC FULLERENE SELF-ASSEMBLY IN HOT CARBON VAPOR. *Nano*, **2007**, 02, 21-30	1.1	15
39	Quantum chemical molecular dynamics study of "shrinking" of hot giant fullerenes. *Journal of Nanoscience and Nanotechnology*, **2007**, 7, 1662-9	1.3	33
38	Parameter Calibration of Transition-Metal Elements for the Spin-Polarized Self-Consistent-Charge Density-Functional Tight-Binding (DFTB) Method: Sc, Ti, Fe, Co, and Ni. *Journal of Chemical Theory and Computation*, **2007**, 3, 1349-67	6.4	177
37	Carbon Nanotubes Grow on the C Face of SiC (0001) during Sublimation Decomposition: Quantum Chemical Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2007**, 111, 12960-12972	3.8	21
36	Modeling carbon nanostructures with the self-consistent charge density-functional tight-binding method: vibrational spectra and electronic structure of C(28), C(60), and C(70). *Journal of Chemical Physics*, **2006**, 125, 214706	3.9	40
35	Origin of the linear relationship between CH2/NH/O-SWNT reaction energies and sidewall curvature: armchair nanotubes. *Journal of the American Chemical Society*, **2006**, 128, 15117-26	16.4	35
34	The C60 formation puzzle "solved": QM/MD simulations reveal the shrinking hot giant road of the dynamic fullerene self-assembly mechanism. *Journal of Physical Chemistry B*, **2006**, 110, 14531-45	3.4	212
33	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, 44702	3.9	18
32	Quantum chemical prediction of reaction pathways and rate constants for dissociative adsorption of CO(x) and NO(x) on the graphite (0001) surface. *Journal of Physical Chemistry B*, **2006**, 110, 21135-44	3.4	36
31	Mechanisms of the reactions of W AND W+ with H2O: computational studies. *Journal of Physical Chemistry A*, **2006**, 110, 4495-501	2.8	8
30	A study of the reaction of N+ with O2: experimental quantification of NO+(a 3Sigma+) production (298-500 K) and computational study of the overall reaction pathways. *Journal of Physical Chemistry A*, **2006**, 110, 3080-6	2.8	5
29	Fe/C interactions during SWNT growth with C2 feedstock molecules: A quantum chemical molecular dynamics study. *Journal of Nanoscience and Nanotechnology*, **2006**, 6, 1259-70	1.3	13
28	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, 10533-8	16.4	156
27	Water clusters on graphite: methodology for quantum chemical a priori prediction of reaction rate constants. *Journal of Physical Chemistry A*, **2005**, 109, 9563-72	2.8	46
26	Performance of the DFTB method in comparison to DFT and semiempirical methods for geometries and energies of C20–C86 fullerene isomers. *Chemical Physics Letters*, **2005**, 412, 210-216	2.5	122

25	High-temperature quantum chemical molecular dynamics simulations of carbon nanostructure self-assembly processes **2005**, 875-889		
24	Towards formation of buckminsterfullerene C60 in quantum chemical molecular dynamics. *Journal of Chemical Physics*, **2005**, 122, 14708	3.9	37
23	Analytical second-order geometrical derivatives of energy for the self-consistent-charge density-functional tight-binding method. *Journal of Chemical Physics*, **2004**, 121, 5163-70	3.9	63
22	Quantum Chemical Molecular Dynamics Model Study of Fullerene Formation from Open-Ended Carbon Nanotubes *Journal of Physical Chemistry A*, **2004**, 108, 3182-3194	2.8	39
21	Oxidation of Alkyl Ions, CnH2n+1+(n= 1), in Reactions with O2and O3in the Gas Phase. *Journal of Physical Chemistry A*, **2004**, 108, 1980-1989	2.8	9
20	From C2 Molecules to Self-Assembled Fullerenes in Quantum Chemical Molecular Dynamics. *Nano Letters*, **2003**, 3, 1657-1664	11.5	79
19	Formation of Fullerene Molecules from Carbon Nanotubes: A Quantum Chemical Molecular Dynamics Study. *Nano Letters*, **2003**, 3, 465-470	11.5	47
18	Ab initio theoretical studies of potential energy surfaces in the photodissociation of the vinyl radical. I. state dissociation. *Journal of Chemical Physics*, **2003**, 119, 6524-6538	3.9	9
17	The internal coordinate path Hamiltonian; application to methanol and malonaldehyde. *Molecular Physics*, **2003**, 101, 3513-3525	1.7	47
16	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	2.8	32
15	ONIOM Study of Ring Opening and Metal Insertion Reactions with Derivatives of C60: Role of Aromaticity in the Opening Process. *Journal of Physical Chemistry A*, **2002**, 106, 680-688	2.8	26
14	Ab initio investigation of the potential energy profiles for the gas phase CH4+O2+(2) reaction system. *Journal of Chemical Physics*, **2001**, 114, 6119-6127	3.9	11
13	Dipole moments of highly vibrationally excited HCN: Theoretical prediction of an experimental diagnostic for delocalized states. *Journal of Chemical Physics*, **2001**, 114, 7923-7934	3.9	33
12	A molecular orbital study on H and H2 elimination pathways from methane, ethane, and propane. *Journal of Chemical Physics*, **2000**, 113, 6139-6148	3.9	14
11	Direct ab initio variational calculation of vibrational energies of the H2O?Cl complex and resolution of experimental differences. *Journal of Chemical Physics*, **2000**, 113, 8401-8403	3.9	61
10	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, 841-8	3	8
9	Ab initio and density functional study on the mechanism of the C2H2++methanol reaction. *Journal of Chemical Physics*, **1999**, 111, 3978-3988	3.9	7
8	Ab initio and density functional study on singlet and triplet states of artemisinin. *Computational and Theoretical Chemistry*, **1998**, 454, 87-90		10

7	Combined ab initio and density functional study on polaron to bipolaron transitions in oligophenyls and oligothiophenes. *Journal of Chemical Physics*, **1997**, 107, 3021-3031	3.9	49
6	Electronic Structure and Properties of Trihalogen Cations X(3)(+) and XY(2)(+) (X, Y = F, Cl, Br, I). *Inorganic Chemistry*, **1996**, 35, 100-109	5.1	13
5	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		21
4	Lithium- and chlorine-doped biphenyl dimers as models for interchain polarons and bipolarons a density functional study. *Chemical Physics Letters*, **1996**, 257, 592-600	2.5	13
3	An ab initio investigation of the charge-transfer complexes of alkali atoms with oligo (P) thiophenes and oligoparaphenylenes: A model calculation on polaronic and bipolaronic defect structures. *Journal of Chemical Physics*, **1995**, 103, 1508-1522	3.9	44
2	Substituent Effects of -NO and -NO2, Groups in Aromatic Systems. *Journal of Organic Chemistry*, **1995**, 60, 6744-6755	4.2	46
1	Quantum Chemistry: Integrated Methods3961-3974		