Stephan Irle

List of Publications by Citations

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	Conjugated organic framework with three-dimensionally ordered stable structure and delocalized clouds. *Nature Communications*, **2013**, 4, 2736	17.4	404
275	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
274	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
273	An n-channel two-dimensional covalent organic framework. *Journal of the American Chemical Society*, **2011**, 133, 14510-3	16.4	277
272	Recent developments in the general atomic and molecular electronic structure system. *Journal of Chemical Physics*, **2020**, 152, 154102	3.9	274
271	Catalytic covalent organic frameworks via pore surface engineering. *Chemical Communications*, **2014**, 50, 1292-4	5.8	243
270	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
269	An ambipolar conducting covalent organic framework with self-sorted and periodic electron donor-acceptor ordering. *Advanced Materials*, **2012**, 24, 3026-31	24	217
268	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
267	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
266	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *Journal of Chemical Physics*, **2020**, 152, 124101	3.9	210
265	Combined experimental and theoretical studies on the photophysical properties of cycloparaphenylenes. *Organic and Biomolecular Chemistry*, **2012**, 10, 5979-84	3.9	202
264	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
263	Rational design of crystalline supermicroporous covalent organic frameworks with triangular topologies. *Nature Communications*, **2015**, 6, 7786	17.4	185
262	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
261	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
260	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

259	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
258	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
257	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
256	Performance of the DFTB method in comparison to DFT and semiempirical methods for geometries and energies of C20□86 fullerene isomers. *Chemical Physics Letters*, **2005**, 412, 210-216	2.5	122
255	Two-dimensional tetrathiafulvalene covalent organic frameworks: towards latticed conductive organic salts. *Chemistry - A European Journal*, **2014**, 20, 14608-13	4.8	109
254	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
253	Large pore donor□cceptor covalent organic frameworks. *Chemical Science*, **2013**, 4, 4505	9.4	100
252	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
251	A New Triazine-Based Covalent Organic Framework for High-Performance Capacitive Energy Storage. *ChemSusChem*, **2017**, 10, 921-929	8.3	88
250	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
249	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
248	Evidence for a new two-dimensional C4H-type polymer based on hydrogenated graphene. *Advanced Materials*, **2011**, 23, 4497-503	24	86
247	QM/MD simulation of SWNT nucleation on transition-metal carbide nanoparticles. *Journal of the American Chemical Society*, **2010**, 132, 15699-707	16.4	86
246	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
245	Comparison of interfacial electron transfer through carboxylate and phosphonate anchoring groups. *Journal of Physical Chemistry A*, **2007**, 111, 6832-42	2.8	84
244	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
243	Designed synthesis of double-stage two-dimensional covalent organic frameworks. *Scientific Reports*, **2015**, 5, 14650	4.9	81
242	Insights into carbon nanotube and graphene formation mechanisms from molecular simulations: a review. *Reports on Progress in Physics*, **2015**, 78, 036501	14.4	80

241	Light-melt adhesive based on dynamic carbon frameworks in a columnar liquid-crystal phase. *Nature Communications*, **2016**, 7, 12094	17.4	79
240	From C2 Molecules to Self-Assembled Fullerenes in Quantum Chemical Molecular Dynamics. *Nano Letters*, **2003**, 3, 1657-1664	11.5	79
239	Growth of carbon nanotubes via twisted graphene nanoribbons. *Nature Communications*, **2013**, 4, 2548	17.4	77
238	Stacked antiaromatic porphyrins. *Nature Communications*, **2016**, 7, 13620	17.4	76
237	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
236	Dimerization-Initiated Preferential Formation of Coronene-Based Graphene Nanoribbons in Carbon Nanotubes. *Journal of Physical Chemistry C*, **2012**, 116, 15141-15145	3.8	74
235	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
234	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
233	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
232	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
231	Hybridization of a flexible cyclooctatetraene core and rigid aceneimide wings for multiluminescent flapping systems. *Chemistry - A European Journal*, **2014**, 20, 2193-200	4.8	68
230	Density-Functional Tight-Binding Combined with the Fragment Molecular Orbital Method. *Journal of Chemical Theory and Computation*, **2014**, 10, 4801-12	6.4	67
229	Growth of Linear Carbon Chains inside Thin Double-Wall Carbon Nanotubes. *Journal of Physical Chemistry C*, **2011**, 115, 13166-13170	3.8	67
228	Origin of the size-dependent fluorescence blueshift in [n]cycloparaphenylenes. *Chemical Science*, **2013**, 4, 187-195	9.4	66
227	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
226	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
225	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
224	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

223	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
222	A femtomolar-range suicide germination stimulant for the parasitic plant. *Science*, **2018**, 362, 1301-1305	33.3	59
221	Zwitterionic Ladder Stilbenes with Phosphonium and Borate Bridges: Intramolecular Cascade Cyclization and Structure–Photophysical Properties Relationship. *Organometallics*, **2011**, 30, 3870-3879	3.8	58
220	RhI-catalyzed aldol-type reaction of organonitriles under mild conditions. *Chemical Communications*, **2008**, 2212-4	5.8	58
219	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
218	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
217	A New Porous Polymer for Highly Efficient Capacitive Energy Storage. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 202-209	8.3	54
216	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
215	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
214	Electrically Activated Conductivity and White Light Emission of a Hydrocarbon Nanoring-Iodine Assembly. *Angewandte Chemie - International Edition*, **2017**, 56, 11196-11202	16.4	49
213	Boosting electrosynthesis of ammonia on surface-engineered MXene Ti3C2. *Nano Energy*, **2020**, 72, 104681	17.1	48
212	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
211	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
210	Formation of Fullerene Molecules from Carbon Nanotubes: A Quantum Chemical Molecular Dynamics Study. *Nano Letters*, **2003**, 3, 465-470	11.5	47
209	The internal coordinate path Hamiltonian; application to methanol and malonaldehyde. *Molecular Physics*, **2003**, 101, 3513-3525	1.7	47
208	Constraint-induced structural deformation of planarized triphenylboranes in the excited state. *Chemical Science*, **2014**, 5, 1296-1304	9.4	46
207	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
206	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

205	Charge Dynamics in A Donor–Acceptor Covalent Organic Framework with Periodically Ordered Bicontinuous Heterojunctions. *Angewandte Chemie*, **2013**, 125, 2071-2075	3.6	46
204	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
203	Substituent Effects of -NO and -NO2, Groups in Aromatic Systems. *Journal of Organic Chemistry*, **1995**, 60, 6744-6755	4.2	46
202	Milestones in molecular dynamics simulations of single-walled carbon nanotube formation: A brief critical review. *Nano Research*, **2009**, 2, 755-767	10	45
201	Cycloparaphenylene as a molecular porous carbon solid with uniform pores exhibiting adsorption-induced softness. *Chemical Science*, **2016**, 7, 4204-4210	9.4	44
200	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
199	Quantum chemical molecular dynamics simulations of dynamic fullerene self-assembly in benzene combustion. *ACS Nano*, **2009**, 3, 2241-57	16.7	44
198	An ab initio investigation of the charge-transfer complexes of alkali atoms with oligo (□) thiophenes and oligoparaphenylenes: A model calculation on polaronic and bipolaronic defect structures. *Journal of Chemical Physics*, **1995**, 103, 1508-1522	3.9	44
197	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
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195	Parametrization and Benchmark of Long-Range Corrected DFTB2 for Organic Molecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 115-125	6.4	41
194	Automatized Parameterization of DFTB Using Particle Swarm Optimization. *Journal of Chemical Theory and Computation*, **2016**, 12, 53-64	6.4	41
193	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
192	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
191	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
190	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
189	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
188	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

187	Regioselectivity control of graphene functionalization by ripples. *Physical Chemistry Chemical Physics*, **2011**, 13, 19449-53	3.6	39
186	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
185	Nucleation of Graphene Precursors on Transition Metal Surfaces: Insights from Theoretical Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 14858-14864	3.8	38
184	Sub-surface nucleation of graphene precursors near a Ni(111) step-edge. *Chemical Communications*, **2012**, 48, 7937-9	5.8	37
183	Towards formation of buckminsterfullerene C60 in quantum chemical molecular dynamics. *Journal of Chemical Physics*, **2005**, 122, 14708	3.9	37
182	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
181	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. *Chemical Science*, **2014**, 5, 3493-3500	9.4	36
180	Dynamics of local chirality during SWCNT growth: armchair versus zigzag nanotubes. *Journal of the American Chemical Society*, **2012**, 134, 9311-9	16.4	36
179	Fullerenes: formation, stability, and reactivity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 350-367	7.9	36
178	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
177	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
176	Topology-Templated Synthesis of Crystalline Porous Covalent Organic Frameworks. *Angewandte Chemie - International Edition*, **2020**, 59, 12162-12169	16.4	34
175	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
174	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
173	Stochastic structure determination for conformationally flexible heterogenous molecular clusters: application to ionic liquids. *Journal of Computational Chemistry*, **2013**, 34, 2591-600	3.5	33
172	Development of Small-Molecule Cryptochrome Stabilizer Derivatives as Modulators of the Circadian Clock. *ChemMedChem*, **2015**, 10, 1489-97	3.7	33
171	Convergence in the evolution of nanodiamond Raman spectra with particle size: a theoretical investigation. *ACS Nano*, **2010**, 4, 4475-86	16.7	33
170	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

169	Quantum chemical molecular dynamics study of "shrinking" of hot giant fullerenes. *Journal of Nanoscience and Nanotechnology*, **2007**, 7, 1662-9	1.3	33
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166	Kinetic Isotope Effect in the Hydrogenation and Deuteration of Graphene. *Advanced Functional Materials*, **2013**, 23, 1628-1635	15.6	32
165	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
164	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
163	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
162	A stacked phenylacetylene dimer. *Physical Chemistry Chemical Physics*, **2011**, 13, 16706-12	3.6	31
161	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
160	Fabrication and optical probing of highly extended, ultrathin graphene nanoribbons in carbon nanotubes. *ACS Nano*, **2015**, 9, 5034-40	16.7	29
159	Two-dimensional artificial light-harvesting antennae with predesigned high-order structure and robust photosensitising activity. *Scientific Reports*, **2016**, 6, 32944	4.9	29
158	Third-order density-functional tight-binding combined with the fragment molecular orbital method. *Chemical Physics Letters*, **2015**, 636, 90-96	2.5	28
157	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
156	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
155	Theoretical insights into chirality-controlled SWCNT growth from a cycloparaphenylene template. *ChemPhysChem*, **2012**, 13, 1479-85	3.2	26
154	Collision-induced fusion of two C60 fullerenes: Quantum chemical molecular dynamics simulations. *Physical Review B*, **2010**, 82,	3.3	26
153	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
152	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

151	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
150	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
149	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
148	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
147	Formation mechanism of polycyclic aromatic hydrocarbons in benzene combustion: Quantum chemical molecular dynamics simulations. *Journal of Chemical Physics*, **2010**, 132, 224303	3.9	24
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145	Theoretical study of cellobiose hydrolysis to glucose in ionic liquids. *Chemical Physics Letters*, **2014**, 603, 7-12	2.5	23
144	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
143	Theoretical Investigation of the Structures and Dynamics of Crystalline Molecular Gyroscopes. *Journal of Physical Chemistry C*, **2012**, 116, 24845-24854	3.8	23
142	Step-edge self-assembly during graphene nucleation on a nickel surface: QM/MD simulations. *Nanoscale*, **2014**, 6, 140-4	7.7	22
141	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
140	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
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138	Pre-Sodiated TiCT MXene Structure and Behavior as Electrode for Sodium-Ion Capacitors. *ACS Nano* , **2021**, 15, 2994-3003	16.7	21
137	Cryptic bioactivity capacitated by synthetic hybrid plant peptides. *Nature Communications*, **2017**, 8, 14318	17.4	20
136	Self-assembly of endohedral metallofullerenes: a decisive role of cooling gas and metal-carbon bonding. *Nanoscale*, **2016**, 8, 3796-808	7.7	20
135	Artificial neural network correction for density-functional tight-binding molecular dynamics simulations. *MRS Communications*, **2019**, 9, 867-873	2.7	20
134	Modeling Charge Transfer in Fullerene Collisions via Real-Time Electron Dynamics. *Journal of Physical Chemistry Letters*, **2012**, 3, 1536-42	6.4	20

133	Polymorphism of [6]Cycloparaphenylene for Packing Structure-dependent Host–Guest Interaction. *Chemistry Letters*, **2017**, 46, 855-857	1.7	19
132	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
131	Glucose transformation to 5-hydroxymethylfurfural in acidic ionic liquid: A quantum mechanical study. *Journal of Computational Chemistry*, **2016**, 37, 327-35	3.5	19
130	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
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128	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
127	QM/MD studies on graphene growth from small islands on the Ni(111) surface. *Nanoscale*, **2016**, 8, 3067-74	7.4	17
126	Critical interpretation of CH- and OH- stretching regions for infrared spectra of methanol clusters (CH3OH)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
125	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
124	Electrically Activated Conductivity and White Light Emission of a Hydrocarbon Nanoring–Iodine Assembly. *Angewandte Chemie*, **2017**, 129, 11348-11354	3.6	16
123	Carbon spiral helix: a nanoarchitecture derived from monovacancy defects in graphene. *Angewandte Chemie - International Edition*, **2010**, 49, 3200-2	16.4	16
122	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
121	Water-mediated deracemization of a bisporphyrin helicate assisted by diastereoselective encapsulation of chiral guests. *Nature Communications*, **2019**, 10, 1457	17.4	15
120	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
119	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
118	Electronic properties of hydrogenated quasi-free-standing graphene. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 2639-2643	1.3	15
117	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
116	Hydroxide Anion Transport in Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2021**, 143, 8970-8975	16.4	15

115	A Macrocyclic Fluorophore Dimer with Flexible Linkers: Bright Excimer Emission with a Long Fluorescence Lifetime. *Angewandte Chemie*, **2016**, 128, 7247-7251	3.6	15
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