Michal Otyepka

List of Publications by Citations

320 papers	17,501 citations	66 h-index	122 g-index
341 ext. papers	20,659 ext. citations	7.9 avg, IF	6.92 L-index

#	Paper	IF	Citations
320	Functionalization of graphene: covalent and non-covalent approaches, derivatives and applications. *Chemical Reviews*, **2012**, 112, 6156-214	68.1	3041
319	Refinement of the Cornell et al. Nucleic Acids Force Field Based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles. *Journal of Chemical Theory and Computation*, **2011**, 7, 2886-2902	6.4	569
318	CAVER: a new tool to explore routes from protein clefts, pockets and cavities. *BMC Bioinformatics*, **2006**, 7, 316	3.6	408
317	Adsorption of small organic molecules on graphene. *Journal of the American Chemical Society*, **2013**, 135, 6372-7	16.4	354
316	Graphitic Nitrogen Triggers Red Fluorescence in Carbon Dots. *ACS Nano*, **2017**, 11, 12402-12410	16.7	351
315	Graphene fluoride: a stable stoichiometric graphene derivative and its chemical conversion to graphene. *Small*, **2010**, 6, 2885-91	11	337
314	Biomimetic Superhydrophobic/Superoleophilic Highly Fluorinated Graphene Oxide and ZIF-8 Composites for Oil-Water Separation. *Angewandte Chemie - International Edition*, **2016**, 55, 1178-82	16.4	295
313	Halogenated graphenes: rapidly growing family of graphene derivatives. *ACS Nano*, **2013**, 7, 6434-64	16.7	291
312	Performance of Molecular Mechanics Force Fields for RNA Simulations: Stability of UUCG and GNRA Hairpins.. *Journal of Chemical Theory and Computation*, **2010**, 6, 3836-3849	6.4	261
311	Stabilizing and Modulating Color by Copigmentation: Insights from Theory and Experiment. *Chemical Reviews*, **2016**, 116, 4937-82	68.1	258
310	Refinement of the Sugar-Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. *Journal of Chemical Theory and Computation*, **2015**, 11, 5723-36	6.4	243
309	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. *Chemical Reviews*, **2018**, 118, 4177-4338	68.1	235
308	Redesigning dehalogenase access tunnels as a strategy for degrading an anthropogenic substrate. *Nature Chemical Biology*, **2009**, 5, 727-33	11.7	207
307	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. *Journal of Chemical Theory and Computation*, **2013**, 9, 2339-2354	6.4	205
306	Assessing the Current State of Amber Force Field Modifications for DNA. *Journal of Chemical Theory and Computation*, **2016**, 12, 4114-27	6.4	203
305	MOLE: a Voronoi diagram-based explorer of molecular channels, pores, and tunnels. *Structure*, **2007** , 15, 1357-63	5.2	189
304	Reference simulations of noncanonical nucleic acids with different variants of the AMBER force field: quadruplex DNA, quadruplex RNA and Z-DNA. *Journal of Chemical Theory and Computation*, **2012**, 8, 2506-2520	6.4	184

303	Photoluminescence effects of graphitic core size and surface functional groups in carbon dots: COO⁻induced red-shift emission. *Carbon*, **2014**, 70, 279-286	10.4	183
302	MOLE 2.0: advanced approach for analysis of biomacromolecular channels. *Journal of Cheminformatics*, **2013**, 5, 39	8.6	183
301	Modelling of graphene functionalization. *Physical Chemistry Chemical Physics*, **2016**, 18, 6351-72	3.6	161
300	Chemistry, properties, and applications of fluorographene. *Applied Materials Today*, **2017**, 9, 60-70	6.6	154
299	Photoluminescent Carbon Nanostructures. *Chemistry of Materials*, **2016**, 28, 4085-4128	9.6	150
298	Graphitic Nitrogen Doping in Carbon Dots Causes Red-Shifted Absorption. *Journal of Physical Chemistry C*, **2016**, 120, 1303-1308	3.8	149
297	Molecular dynamics and quantum mechanics of RNA: conformational and chemical change we can believe in. *Accounts of Chemical Research*, **2010**, 43, 40-7	24.3	140
296	Doping with Graphitic Nitrogen Triggers Ferromagnetism in Graphene. *Journal of the American Chemical Society*, **2017**, 139, 3171-3180	16.4	124
295	Band Gaps and Optical Spectra of Chlorographene, Fluorographene and Graphane from G0W0, GW0 and GW Calculations on Top of PBE and HSE06 Orbitals. *Journal of Chemical Theory and Computation*, **2013**, 9, 4155-64	6.4	115
294	Membrane position of ibuprofen agrees with suggested access path entrance to cytochrome P450 2C9 active site. *Journal of Physical Chemistry A*, **2011**, 115, 11248-55	2.8	114
293	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. *Journal of Physical Chemistry Letters*, **2014**, 5, 1771-82	6.4	113
292	MOLEonline: a web-based tool for analyzing channels, tunnels and pores (2018 update). *Nucleic Acids Research*, **2018**, 46, W368-W373	20.1	112
291	Base Pair Fraying in Molecular Dynamics Simulations of DNA and RNA. *Journal of Chemical Theory and Computation*, **2014**, 10, 3177-89	6.4	106
290	What common structural features and variations of mammalian P450s are known to date?. *Biochimica Et Biophysica Acta - General Subjects*, **2007**, 1770, 376-89	4	102
289	Cyanographene and Graphene Acid: Emerging Derivatives Enabling High-Yield and Selective Functionalization of Graphene. *ACS Nano*, **2017**, 11, 2982-2991	16.7	99
288	Flexibility of human cytochromes P450: molecular dynamics reveals differences between CYPs 3A4, 2C9, and 2A6, which correlate with their substrate preferences. *Journal of Physical Chemistry B*, **2008**, 112, 8165-73	3.4	97
287	MOLEonline 2.0: interactive web-based analysis of biomacromolecular channels. *Nucleic Acids Research*, **2012**, 40, W222-7	20.1	96
286	Positioning of antioxidant quercetin and its metabolites in lipid bilayer membranes: implication for their lipid-peroxidation inhibition. *Journal of Physical Chemistry B*, **2012**, 116, 1309-18	3.4	95

285	Band gaps and structural properties of graphene halides and their derivates: a hybrid functional study with localized orbital basis sets. *Journal of Chemical Physics*, **2012**, 137, 034709	3.9	93
284	The Nature of the Binding of Au, Ag, and Pd to Benzene, Coronene, and Graphene: From Benchmark CCSD(T) Calculations to Plane-Wave DFT Calculations. *Journal of Chemical Theory and Computation*, **2011**, 7, 3743-3755	6.4	90
283	Anaerobic Reaction of Nanoscale Zerovalent Iron with Water: Mechanism and Kinetics. *Journal of Physical Chemistry C*, **2014**, 118, 13817-13825	3.8	87
282	Environmental applications of chemically pure natural ferrihydrite. *Environmental Science & Technology*, **2007**, 41, 4367-74	10.3	86
281	Room temperature organic magnets derived from sp functionalized graphene. *Nature Communications*, **2017**, 8, 14525	17.4	81
280	Reactivity of Fluorographene: A Facile Way toward Graphene Derivatives. *Journal of Physical Chemistry Letters*, **2015**, 6, 1430-4	6.4	81
279	Convergence of Free Energy Profile of Coumarin in Lipid Bilayer. *Journal of Chemical Theory and Computation*, **2012**, 8, 1200-1211	6.4	81
278	Nature and magnitude of aromatic base stacking in DNA and RNA: Quantum chemistry, molecular mechanics, and experiment. *Biopolymers*, **2013**, 99, 978-88	2.2	80
277	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. *Journal of Chemical Theory and Computation*, **2013**, 9, 4287-92	6.4	80
276	A high efficiency H2S gas sensor material: paper like Fe2O3/graphene nanosheets and structural alignment dependency of device efficiency. *Journal of Materials Chemistry A*, **2014**, 2, 6714-6717	13	79
275	Behavior of human cytochromes P450 on lipid membranes. *Journal of Physical Chemistry B*, **2013**, 117, 11556-64	3.4	79
274	Spectroscopic Fingerprints of Graphitic, Pyrrolic, Pyridinic, and Chemisorbed Nitrogen in N-Doped Graphene. *Journal of Physical Chemistry C*, **2019**, 123, 10695-10702	3.8	78
273	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. *Journal of Chemical Theory and Computation*, **2016**, 12, 4534-48	6.4	77
272	Hydrophobic Metal-Organic Frameworks. *Advanced Materials*, **2019**, 31, e1900820	24	76
271	Mixed-Valence Single-Atom Catalyst Derived from Functionalized Graphene. *Advanced Materials*, **2019**, 31, e1900323	24	76
270	Crystal structure of haloalkane dehalogenase LinB from Sphingomonas paucimobilis UT26 at 0.95 A resolution: dynamics of catalytic residues. *Biochemistry*, **2004**, 43, 870-8	3.2	76
269	Amphiphilic drug-like molecules accumulate in a membrane below the head group region. *Journal of Physical Chemistry B*, **2014**, 118, 1030-9	3.4	75
268	Semiempirical quantum mechanical method PM6-DH2X describes the geometry and energetics of CK2-inhibitor complexes involving halogen bonds well, while the empirical potential fails. *Journal of Physical Chemistry B*, **2011**, 115, 8581-9	3.4	75

267	Explicit Water Models Affect the Specific Solvation and Dynamics of Unfolded Peptides While the Conformational Behavior and Flexibility of Folded Peptides Remain Intact. *Journal of Chemical Theory and Computation*, **2010**, 6, 3569-79	6.4	75
266	Thiofluorographene-hydrophilic graphene derivative with semiconducting and genosensing properties. *Advanced Materials*, **2015**, 27, 2305-10	24	74
265	Nature of Absorption Bands in Oxygen-Functionalized Graphitic Carbon Dots. *Journal of Physical Chemistry C*, **2015**, 119, 13369-13373	3.8	74
264	Theoretical studies of RNA catalysis: hybrid QM/MM methods and their comparison with MD and QM. *Methods*, **2009**, 49, 202-16	4.6	74
263	Human virus detection with graphene-based materials. *Biosensors and Bioelectronics*, **2020**, 166, 112436	11.8	74
262	Extensive molecular dynamics simulations showing that canonical G8 and protonated A38H+ forms are most consistent with crystal structures of hairpin ribozyme. *Journal of Physical Chemistry B*, **2010**, 114, 6642-52	3.4	72
261	Activation and inhibition of cyclin-dependent kinase-2 by phosphorylation; a molecular dynamics study reveals the functional importance of the glycine-rich loop. *Protein Science*, **2004**, 13, 1449-57	6.3	72
260	Shape-Assisted 2D MOF/Graphene Derived Hybrids as Exceptional Lithium-Ion Battery Electrodes. *Advanced Functional Materials*, **2019**, 29, 1902539	15.6	71
259	Quaternized carbon dot-modified graphene oxide for selective cell labelling--controlled nucleus and cytoplasm imaging. *Chemical Communications*, **2014**, 50, 10782-5	5.8	70
258	Computer Folding of RNA Tetraloops? Are We There Yet?. *Journal of Chemical Theory and Computation*, **2013**, 9, 2115-25	6.4	69
257	Chemical nature of boron and nitrogen dopant atoms in graphene strongly influences its electronic properties. *Physical Chemistry Chemical Physics*, **2014**, 16, 14231-5	3.6	68
256	The DNA and RNA sugar-phosphate backbone emerges as the key player. An overview of quantum-chemical, structural biology and simulation studies. *Physical Chemistry Chemical Physics*, **2012**, 14, 15257-77	3.6	68
255	Sulfur Doping Induces Strong Ferromagnetic Ordering in Graphene: Effect of Concentration and Substitution Mechanism. *Advanced Materials*, **2016**, 28, 5045-53	24	67
254	Folding of guanine quadruplex molecules-funnel-like mechanism or kinetic partitioning? An overview from MD simulation studies. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 1246-1263	4	66
253	Large-scale compensation of errors in pairwise-additive empirical force fields: comparison of AMBER intermolecular terms with rigorous DFT-SAPT calculations. *Physical Chemistry Chemical Physics*, **2010**, 12, 10476-93	3.6	65
252	Membrane-attached mammalian cytochromes P450: An overview of the membrane's effects on structure, drug binding, and interactions with redox partners. *Journal of Inorganic Biochemistry*, **2018**, 183, 117-136	4.2	64
251	Dependence of A-RNA simulations on the choice of the force field and salt strength. *Physical Chemistry Chemical Physics*, **2009**, 11, 10701-11	3.6	62
250	Benchmarking of Force Fields for Molecule-Membrane Interactions. *Journal of Chemical Theory and Computation*, **2014**, 10, 4143-51	6.4	61

249	Anatomy of enzyme channels. *BMC Bioinformatics*, **2014**, 15, 379	3.6	61
248	Force-field dependence of chignolin folding and misfolding: comparison with experiment and redesign. *Biophysical Journal*, **2012**, 102, 1897-906	2.9	61
247	Quantification of the interaction forces between metals and graphene by quantum chemical calculations and dynamic force measurements under ambient conditions. *ACS Nano*, **2013**, 7, 1646-51	16.7	60
246	Simulations of A-RNA duplexes. The effect of sequence, solute force field, water model, and salt concentration. *Journal of Physical Chemistry B*, **2012**, 116, 9899-916	3.4	58
245	Docking-based development of purine-like inhibitors of cyclin-dependent kinase-2. *Journal of Medicinal Chemistry*, **2000**, 43, 2506-13	8.3	58
244	Is Single Layer MoS Stable in the Air?. *Chemistry - A European Journal*, **2017**, 23, 13233-13239	4.8	57
243	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. *Journal of Chemical Theory and Computation*, **2019**, 15, 3288-3305	6.4	56
242	Fluorinated graphenes as advanced biosensors - effect of fluorine coverage on electron transfer properties and adsorption of biomolecules. *Nanoscale*, **2016**, 8, 12134-42	7.7	56
241	Hydrophilic Nanotube Supported Graphene□Water Dispersible Carbon Superstructure with Excellent Conductivity. *Advanced Functional Materials*, **2015**, 25, 1481-1487	15.6	56
240	Can We Accurately Describe the Structure of Adenine Tracts in B-DNA? Reference Quantum-Chemical Computations Reveal Overstabilization of Stacking by Molecular Mechanics. *Journal of Chemical Theory and Computation*, **2012**, 8, 2448-60	6.4	56
239	High-Yield Alkylation and Arylation of Graphene via Grignard Reaction with Fluorographene. *Chemistry of Materials*, **2017**, 29, 926-930	9.6	55
238	Can We Execute Stable Microsecond-Scale Atomistic Simulations of Protein-RNA Complexes?. *Journal of Chemical Theory and Computation*, **2015**, 11, 1220-43	6.4	53
237	Protonation states of the key active site residues and structural dynamics of the glmS riboswitch as revealed by molecular dynamics. *Journal of Physical Chemistry B*, **2010**, 114, 8701-12	3.4	53
236	Is there a relationship between the substrate preferences and structural flexibility of cytochromes P450?. *Current Drug Metabolism*, **2012**, 13, 130-42	3.5	53
235	Non-covalent control of spin-state in metal-organic complex by positioning on N-doped graphene. *Nature Communications*, **2018**, 9, 2831	17.4	52
234	Covalent Graphene-MOF Hybrids for High-Performance Asymmetric Supercapacitors. *Advanced Materials*, **2021**, 33, e2004560	24	51
233	Synergism of antioxidant action of vitamins E, C and quercetin is related to formation of molecular associations in biomembranes. *Chemical Communications*, **2015**, 51, 7713-6	5.8	50
232	Water dispersible functionalized graphene fluoride with significant nonlinear optical response. *Chemical Physics Letters*, **2012**, 543, 101-105	2.5	50

231	In silico structural and functional analysis of fragments of the ankyrin repeat protein p18(INK4c). *Journal of Biomolecular Structure and Dynamics*, **2010**, 27, 521-40	3.6	49
230	Identification of tunnels in proteins, nucleic acids, inorganic materials and molecular ensembles. *Biotechnology Journal*, **2007**, 2, 62-7	5.6	49
229	Comparison of ab Initio, DFT, and Semiempirical QM/MM Approaches for Description of Catalytic Mechanism of Hairpin Ribozyme. *Journal of Chemical Theory and Computation*, **2014**, 10, 1608-22	6.4	48
228	Transferable scoring function based on semiempirical quantum mechanical PM6-DH2 method: CDK2 with 15 structurally diverse inhibitors. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 223-35	4.2	46
227	Reactivity of fluorographene is triggered by point defects: beyond the perfect 2D world. *Nanoscale*, **2018**, 10, 4696-4707	7.7	45
226	Molecular insight into affinities of drugs and their metabolites to lipid bilayers. *Journal of Physical Chemistry B*, **2013**, 117, 2403-10	3.4	45
225	Flexibility of human cytochrome P450 enzymes: molecular dynamics and spectroscopy reveal important function-related variations. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2011**, 1814, 58-68	4	45
224	The surface and structural properties of graphite fluoride. *Carbon*, **2015**, 94, 804-809	10.4	44
223	Understanding RNA Flexibility Using Explicit Solvent Simulations: The Ribosomal and Group I Intron Reverse Kink-Turn Motifs. *Journal of Chemical Theory and Computation*, **2011**, 7, 2963-80	6.4	43
222	Dynamics and hydration of the active sites of mammalian cytochromes P450 probed by molecular dynamics simulations. *Current Drug Metabolism*, **2012**, 13, 177-89	3.5	43
221	Band gaps and optical spectra from single- and double-layer fluorographene to graphite fluoride: many-body effects and excitonic states. *Annalen Der Physik*, **2014**, 526, 408-414	2.6	42
220	Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy. *Physical Chemistry Chemical Physics*, **2014**, 16, 20915-23	3.6	42
219	Effect of Monovalent Ion Parameters on Molecular Dynamics Simulations of G-Quadruplexes. *Journal of Chemical Theory and Computation*, **2017**, 13, 3911-3926	6.4	42
218	How to understand atomistic molecular dynamics simulations of RNA and protein-RNA complexes?. *Wiley Interdisciplinary Reviews RNA*, **2017**, 8, e1405	9.3	42
217	General base catalysis for cleavage by the active-site cytosine of the hepatitis delta virus ribozyme: QM/MM calculations establish chemical feasibility. *Journal of Physical Chemistry B*, **2008**, 112, 11177-87	3.4	42
216	Covalently functionalized graphene as a supercapacitor electrode material. *FlatChem*, **2019**, 13, 25-33	5.1	42
215	Malonate-based inhibitors of mammalian serine racemase: kinetic characterization and structure-based computational study. *European Journal of Medicinal Chemistry*, **2015**, 89, 189-97	6.8	41
214	Fluorographites (CF(x))n exhibit improved heterogeneous electron-transfer rates with increasing level of fluorination: towards the sensing of biomolecules. *Chemistry - A European Journal*, **2014**, 20, 6665-71	4.8	41

213	Molecular mechanism of preQ1 riboswitch action: a molecular dynamics study. *Journal of Physical Chemistry B*, **2012**, 116, 12721-34	3.4	40
212	Different mechanisms of CDK5 and CDK2 activation as revealed by CDK5/p25 and CDK2/cyclin A dynamics. *Journal of Biological Chemistry*, **2006**, 281, 7271-81	5.4	40
211	Insights into Stability and Folding of GNRA and UNCG Tetraloops Revealed by Microsecond Molecular Dynamics and Well-Tempered Metadynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 3866-77	6.4	39
210	Structural Changes in Ceramide Bilayers Rationalize Increased Permeation through Stratum Corneum Models with Shorter Acyl Tails. *Journal of Physical Chemistry B*, **2015**, 119, 9811-9	3.4	39
209	Organic adsorbates have higher affinities to fluorographene than to graphene. *Applied Materials Today*, **2016**, 5, 142-149	6.6	39
208	Functional Nanosheet Synthons by Covalent Modification of Transition-Metal Dichalcogenides. *Chemistry of Materials*, **2017**, 29, 2066-2073	9.6	38
207	Interaction of Graphene and Arenes with Noble Metals. *Journal of Physical Chemistry C*, **2012**, 116, 14151-14162	3.8	38
206	Hairpins participating in folding of human telomeric sequence quadruplexes studied by standard and T-REMD simulations. *Nucleic Acids Research*, **2015**, 43, 9626-44	20.1	37
205	How to understand quantum chemical computations on DNA and RNA systems? A practical guide for non-specialists. *Methods*, **2013**, 64, 3-11	4.6	37
204	Random Phase Approximation in Surface Chemistry: Water Splitting on Iron. *Journal of Chemical Theory and Computation*, **2013**, 9, 3670-6	6.4	37
203	The nature of high surface energy sites in graphene and graphite. *Carbon*, **2014**, 73, 448-453	10.4	36
202	Role of Enzyme Flexibility in Ligand Access and Egress to Active Site: Bias-Exchange Metadynamics Study of 1,3,7-Trimethyluric Acid in Cytochrome P450 3A4. *Journal of Chemical Theory and Computation*, **2016**, 12, 2101-9	6.4	35
201	Lipid Enhanced Exfoliation for Production of Graphene Nanosheets. *Journal of Physical Chemistry C*, **2013**, 117, 11800-11803	3.8	35
200	Functionally relevant motions of haloalkane dehalogenases occur in the specificity-modulating cap domains. *Protein Science*, **2002**, 11, 1206-1217	6.3	35
199	Adsorption of Organic Molecules to van der Waals Materials: Comparison of Fluorographene and Fluorographite with Graphene and Graphite. *Journal of Chemical Theory and Computation*, **2017**, 13, 1328-1340	6.4	34
198	2D Chemistry: Chemical Control of Graphene Derivatization. *Journal of Physical Chemistry Letters*, **2018**, 9, 3580-3585	6.4	34
197	The mechanism of inhibition of the cyclin-dependent kinase-2 as revealed by the molecular dynamics study on the complex CDK2 with the peptide substrate HHASPRK. *Protein Science*, **2005**, 14, 445-51	6.3	34
196	Effect of guanine to inosine substitution on stability of canonical DNA and RNA duplexes: molecular dynamics thermodynamics integration study. *Journal of Physical Chemistry B*, **2013**, 117, 1872-9	3.4	33

195	In silico pharmacology: Drug membrane partitioning and crossing. *Pharmacological Research*, **2016**, 111, 471-486	10.2	33
194	High-Performance Supercapacitors Based on a Zwitterionic Network of Covalently Functionalized Graphene with Iron Tetraaminophthalocyanine. *Advanced Functional Materials*, **2018**, 28, 1801111	15.6	32
193	Exact roles of individual chemical forms of nitrogen in the photoluminescent properties of nitrogen-doped carbon dots. *Applied Materials Today*, **2017**, 7, 190-200	6.6	31
192	Reactive conformation of the active site in the hairpin ribozyme achieved by molecular dynamics simulations with ∆∆force field reparametrizations. *Journal of Physical Chemistry B*, **2015**, 119, 4220-9	3.4	31
191	Exploring the Dynamics of Propeller Loops in Human Telomeric DNA Quadruplexes Using Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 2458-2480	6.4	30
190	Dichlorocarbene-Functionalized Fluorographene: Synthesis and Reaction Mechanism. *Small*, **2015**, 11, 3790-6	11	30
189	Accurate surface energies from first principles. *Physical Review B*, **2015**, 91,	3.3	30
188	QM/MM studies of hairpin ribozyme self-cleavage suggest the feasibility of multiple competing reaction mechanisms. *Journal of Physical Chemistry B*, **2011**, 115, 13911-24	3.4	30
187	Structure, dynamical stability, and electronic properties of phases in TaS2 from a high-level quantum mechanical calculation. *Physical Review B*, **2015**, 92,	3.3	29
186	Immobilized Enzymes on Graphene as Nanobiocatalyst. *ACS Applied Materials & Interfaces*, **2020**, 12, 250-259	9.5	29
185	Interaction of single- and double-stranded DNA with multilayer MXene by fluorescence spectroscopy and molecular dynamics simulations. *Chemical Science*, **2019**, 10, 10010-10017	9.4	29
184	Are Waters around RNA More than Just a Solvent? - An Insight from Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 401-11	6.4	28
183	Antiallergic effects of pigments isolated from green sea urchin (Strongylocentrotus droebachiensis) shells. *Planta Medica*, **2013**, 79, 1698-704	3.1	28
182	Functional flexibility of human cyclin-dependent kinase-2 and its evolutionary conservation. *Protein Science*, **2008**, 17, 22-33	6.3	28
181	Role of the Edge Properties in the Hydrogen Evolution Reaction on MoS. *Chemistry - A European Journal*, **2017**, 23, 4863-4869	4.8	27
180	The Role of Protein-Protein and Protein-Membrane Interactions on P450 Function. *Drug Metabolism and Disposition*, **2016**, 44, 576-90	4	27
179	NZVI modified magnetic filter paper with high redox and catalytic activities for advanced water treatment technologies. *Chemical Communications*, **2014**, 50, 15673-6	5.8	27
178	Choosing a density functional for modeling adsorptive hydrogen storage: reference quantum mechanical calculations and a comparison of dispersion-corrected density functionals. *Physical Chemistry Chemical Physics*, **2015**, 17, 6423-32	3.6	27

177	Density-functional, density-functional tight-binding, and wave function calculations on biomolecular systems. *Journal of Physical Chemistry A*, **2007**, 111, 5642-7	2.8	26
176	Influence of BII Backbone Substates on DNA Twist: A Unified View and Comparison of Simulation and Experiment for All 136 Distinct Tetranucleotide Sequences. *Journal of Chemical Information and Modeling*, **2017**, 57, 275-287	6.1	25
175	Interplay between Ethanol Adsorption to High-Energy Sites and Clustering on Graphene and Graphite Alters the Measured Isosteric Adsorption Enthalpies. *Journal of Physical Chemistry C*, **2015**, 119, 20535-20543	3.8	25
174	Dissociation of Water at Iron Surfaces: Generalized Gradient Functional and Range-Separated Hybrid Functional Study. *Journal of Physical Chemistry C*, **2012**, 116, 25470-25477	3.8	25
173	Benchmark quantum-chemical calculations on a complete set of rotameric families of the DNA sugar-phosphate backbone and their comparison with modern density functional theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 7295-310	3.6	25
172	Noncanonical hydrogen bonding in nucleic acids. Benchmark evaluation of key base-phosphate interactions in folded RNA molecules using quantum-chemical calculations and molecular dynamics simulations. *Journal of Physical Chemistry A*, **2011**, 115, 11277-92	2.8	25
171	Mechanism of enhanced conversion of 1,2,3-trichloropropane by mutant haloalkane dehalogenase revealed by molecular modeling. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 375-83	4.2	25
170	Structural Dynamics of Carbon Dots in Water and N, N-Dimethylformamide Probed by All-Atom Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 2076-2083	6.4	24
169	Parallel G-triplexes and G-hairpins as potential transitory ensembles in the folding of parallel-stranded DNA G-Quadruplexes. *Nucleic Acids Research*, **2019**, 47, 7276-7293	20.1	24
168	Second step of hydrolytic dehalogenation in haloalkane dehalogenase investigated by QM/MM methods. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 707-17	4.2	24
167	Dynamics and binding modes of free cdk2 and its two complexes with inhibitors studied by computer simulations. *Journal of Biomolecular Structure and Dynamics*, **2002**, 20, 141-54	3.6	24
166	Recent Progress in Emerging Two-Dimensional Transition Metal Carbides. *Nano-Micro Letters*, **2021**, 13, 183	19.5	24
165	Optical properties of wine pigments: theoretical guidelines with new methodological perspectives. *Tetrahedron*, **2015**, 71, 3079-3088	2.4	23
164	Role of the puckered anisotropic surface in the surface and adsorption properties of black phosphorus. *Nanoscale*, **2018**, 10, 8979-8988	7.7	23
163	Palladium nanoparticles supported on graphene acid: a stable and eco-friendly bifunctional C□ homo- and cross-coupling catalyst. *Green Chemistry*, **2019**, 21, 5238-5247	10	23
162	A Novel Approach for Deriving Force Field Torsion Angle Parameters Accounting for Conformation-Dependent Solvation Effects. *Journal of Chemical Theory and Computation*, **2012**, 8, 3232-42	6.4	23
161	ATP and magnesium drive conformational changes of the Na+/K+-ATPase cytoplasmic headpiece. *Biochimica Et Biophysica Acta - Biomembranes*, **2009**, 1788, 1081-91	3.8	23
160	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. *Applied Materials Today*, **2021**, 22, 100924	6.6	23

159	Noncanonical αβ Backbone Conformations in RNA and the Accuracy of Their Description by the AMBER Force Field. *Journal of Physical Chemistry B*, **2017**, 121, 2420-2433	3.4	22
158	The role of an active site Mg(2+) in HDV ribozyme self-cleavage: insights from QM/MM calculations. *Physical Chemistry Chemical Physics*, **2015**, 17, 670-9	3.6	22
157	Positive and Negative Effects of Dopants toward Electrocatalytic Activity of MoS and WS: Experiments and Theory. *ACS Applied Materials & Interfaces*, **2020**, 12, 20383-20392	9.5	22
156	ChannelsDB: database of biomacromolecular tunnels and pores. *Nucleic Acids Research*, **2018**, 46, D399-D405	2015	22
155	Rationalization of reduced penetration of drugs through ceramide gel phase membrane. *Langmuir*, **2014**, 30, 13942-8	4	22
154	Surface heterogeneity: Information from inverse gas chromatography and application to model pharmaceutical substances. *Current Opinion in Colloid and Interface Science*, **2016**, 24, 64-71	7.6	22
153	First Step in the Reaction of Zerovalent Iron with Water. *Journal of Chemical Theory and Computation*, **2011**, 7, 2876-85	6.4	21
152	Glycine-rich loop of mitochondrial processing peptidase alpha-subunit is responsible for substrate recognition by a mechanism analogous to mitochondrial receptor Tom20. *Journal of Molecular Biology*, **2010**, 396, 1197-210	6.5	21
151	Interaction energies for the purine inhibitor roscovitine with cyclin-dependent kinase 2: correlated ab initio quantum-chemical, DFT and empirical calculations. *Chemistry - A European Journal*, **2006**, 12, 4297-304	4.8	21
150	2,6,8,9-tetrasubstituted purines as new CDK1 inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2003**, 13, 2993-6	2.9	21
149	Surface energy analysis (SEA) and rheology of powder milk dairy products. *Food Chemistry*, **2015**, 174, 25-30	8.5	20
148	Energies and 2′-Hydroxyl Group Orientations of RNA Backbone Conformations. Benchmark CCSD(T)/CBS Database, Electronic Analysis, and Assessment of DFT Methods and MD Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 463-80	6.4	20
147	Coarse-grain simulations of skin ceramide NS with newly derived parameters clarify structure of melted phase. *Journal of Physical Chemistry B*, **2015**, 119, 3988-98	3.4	20
146	Lipid bilayer membrane affinity rationalizes inhibition of lipid peroxidation by a natural lignan antioxidant. *Journal of Physical Chemistry B*, **2013**, 117, 5043-9	3.4	20
145	Noncovalent Integration of a Bioinspired Ni Catalyst to Graphene Acid for Reversible Electrocatalytic Hydrogen Oxidation. *ACS Applied Materials & Interfaces*, **2020**, 12, 5805-5811	9.5	20
144	Chemical Tuning of Specific Capacitance in Functionalized Fluorographene. *Chemistry of Materials*, **2019**, 31, 4698-4709	9.6	19
143	Binding of quinidine radically increases the stability and decreases the flexibility of the cytochrome P450 2D6 active site. *Journal of Inorganic Biochemistry*, **2012**, 110, 46-50	4.2	19
142	The Hallmarks of Copper Single Atom Catalysts in Direct Alcohol Fuel Cells and Electrochemical CO2 Fixation. *Advanced Materials Interfaces*, **2021**, 8, 2001822	4.6	19

141	Spin-Crossing in an Organometallic Pt-Benzene Complex. *Journal of Chemical Theory and Computation*, **2013**, 9, 1461-8	6.4	18
140	Structural dynamics of propeller loop: towards folding of RNA G-quadruplex. *Nucleic Acids Research* , **2018**, 46, 8754-8771	20.1	18
139	Molecular dynamic simulations of protein/RNA complexes: CRISPR/Csy4 endoribonuclease. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 1072-1090	4	17
138	Tunable Synthesis of Nitrogen Doped Graphene from Fluorographene under Mild Conditions. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 4764-4772	8.3	17
137	Cyanographene and Graphene Acid: The Functional Group of Graphene Derivative Determines the Application in Electrochemical Sensing and Capacitors. *ChemElectroChem*, **2019**, 6, 229-234	4.3	17
136	Intrinsic photoluminescence of amine-functionalized graphene derivatives for bioimaging applications. *Applied Materials Today*, **2019**, 17, 112-122	6.6	17
135	Direct mapping of chemical oxidation of individual graphene sheets through dynamic force measurements at the nanoscale. *Nanoscale*, **2017**, 9, 119-127	7.7	17
134	Conformational Energies of DNA Sugar−Phosphate Backbone: Reference QM Calculations and a Comparison with Density Functional Theory and Molecular Mechanics. *Journal of Chemical Theory and Computation*, **2010**, 6, 3817-3835	6.4	17
133	Analysis of CDK2 active-site hydration: a method to design new inhibitors. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 258-74	4.2	17
132	Effect of Lipid Charge on Membrane Immersion of Cytochrome P450 3A4. *Journal of Physical Chemistry B*, **2016**, 120, 11205-11213	3.4	17
131	Arene CH insertion catalyzed by ferrocene covalently heterogenized on graphene acid. *Carbon*, **2019**, 143, 318-328	10.4	17
130	Microsecond-Scale MD Simulations of HIV-1 DIS Kissing-Loop Complexes Predict Bulged-In Conformation of the Bulged Bases and Reveal Interesting Differences between Available Variants of the AMBER RNA Force Fields. *Journal of Physical Chemistry B*, **2015**, 119, 15176-90	3.4	16
129	Metal Halide Perovskite@Metal-Organic Framework Hybrids: Synthesis, Design, Properties, and Applications. *Small*, **2020**, 16, e2004891	11	16
128	Single Co-Atoms as Electrocatalysts for Efficient Hydrazine Oxidation Reaction. *Small*, **2021**, 17, e2006477	11	16
127	Alkynylation of graphene via the Sonogashira C-C cross-coupling reaction on fluorographene. *Chemical Communications*, **2019**, 55, 1088-1091	5.8	15
126	Fine-Tuning of the AMBER RNA Force Field with a New Term Adjusting Interactions of Terminal Nucleotides. *Journal of Chemical Theory and Computation*, **2020**, 16, 3936-3946	6.4	15
125	Disparate HDV ribozyme crystal structures represent intermediates on a rugged free-energy landscape. *Rna*, **2014**, 20, 1112-28	5.8	15
124	Surface properties of MoS probed by inverse gas chromatography and their impact on electrocatalytic properties. *Nanoscale*, **2017**, 9, 19236-19244	7.7	15

123	Effect of cholesterol on the structure of membrane-attached cytochrome P450 3A4. *Journal of Chemical Information and Modeling*, **2015**, 55, 628-35	6.1	15
122	A cancer-derived mutation in the PSTAIRE helix of cyclin-dependent kinase 2 alters the stability of cyclin binding. *Biochimica Et Biophysica Acta - Molecular Cell Research*, **2010**, 1803, 858-64	4.9	15
121	Unique cellular network formation guided by heterostructures based on reduced graphene oxide - TiCT MXene hydrogels. *Acta Biomaterialia*, **2020**, 115, 104-115	10.8	15
120	Ion Interactions across Graphene in Electrolyte Aqueous Solutions. *Journal of Physical Chemistry C*, **2019**, 123, 9799-9806	3.8	14
119	Functionally relevant motions of haloalkane dehalogenases occur in the specificity-modulating cap domains. *Protein Science*, **2002**, 11, 1206-17	6.3	14
118	Carbon Dots Detect Water-to-Ice Phase Transition and Act as Alcohol Sensors Fluorescence Turn-Off/On Mechanism. *ACS Nano*, **2021**, 15, 6582-6593	16.7	14
117	Variability of C Bonds Governs the Formation of Specific Structural Motifs in Fluorinated Graphenes. *Journal of Physical Chemistry C*, **2019**, 123, 27896-27903	3.8	13
116	Combined high degree of carboxylation and electronic conduction in graphene acid sets new limits for metal free catalysis in alcohol oxidation. *Chemical Science*, **2019**, 10, 9438-9445	9.4	13
115	Conformational Behavior and Optical Properties of a Fluorophore Dimer as a Model of Luminescent Centers in Carbon Dots. *Journal of Physical Chemistry C*, **2020**, 124, 14327-14337	3.8	13
114	Correlation of Dissociation Constants of 2- and 2,6-Substituted Anilines in Water by Methods Based on the Similarity Principle and Quantum-Chemistry Calculations. *Journal of Physical Chemistry A*, **2003**, 107, 11489-11496	2.8	13
113	Silver Covalently Bound to Cyanographene Overcomes Bacterial Resistance to Silver Nanoparticles and Antibiotics. *Advanced Science*, **2021**, 8, 2003090	13.6	13
112	A- to B-DNA Transition in AMBER Force Fields and Its Coupling to Sugar Pucker. *Journal of Chemical Theory and Computation*, **2018**, 14, 319-328	6.4	13
111	Bonding Motifs in Metal-Organic Compounds on Surfaces. *Journal of the American Chemical Society*, **2018**, 140, 12884-12889	16.4	13
110	Nonenzymatic Oligomerization of 3N,5NCyclic CMP Induced by Proton and UV Irradiation Hints at a Nonfastidious Origin of RNA. *ChemBioChem*, **2017**, 18, 1535-1543	3.8	12
109	Theoretical studies on the intermolecular interactions of potentially primordial base-pair analogues. *Chemistry - A European Journal*, **2010**, 16, 3057-65	4.8	12
108	Tailoring conjugation and vibrational modes to steer on-surface synthesis of pentalene-bridged ladder polymers. *Nature Communications*, **2020**, 11, 4567	17.4	12
107	Biomimetische superhydrophobe/superoleophile hoch fluorierte Graphenoxid-ZIF-8-Komposite f die Wasser-Trennung. *Angewandte Chemie*, **2016**, 128, 1193-1197	3.6	12
106	Multidrug resistance-associated protein 4 (MRP4) controls ganciclovir intracellular accumulation and contributes to ganciclovir-induced neutropenia in renal transplant patients. *Pharmacological Research*, **2016**, 111, 501-508	10.2	12

105	Selective Functionalization Blended with Scaffold Conductivity in Graphene Acid Promotes HO Electrochemical Sensing. *ACS Omega*, **2019**, 4, 19944-19952	3.9	12
104	Thiophenol-Modified Fluorographene Derivatives for Nonlinear Optical Applications. *ChemPlusChem*, **2019**, 84, 1288-1298	2.8	11
103	Structural patterns of the human ABCC4/MRP4 exporter in lipid bilayers rationalize clinically observed polymorphisms. *Pharmacological Research*, **2018**, 133, 318-327	10.2	11
102	Challenges in the theoretical description of nanoparticle reactivity: Nano zero-valent iron. *International Journal of Quantum Chemistry*, **2014**, 114, 987-992	2.1	11
101	Molecular insights into the role of a distal F240A mutation that alters CYP1A1 activity towards persistent organic pollutants. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 2852-2860	4	11
100	A computational study of the glycine-rich loop of mitochondrial processing peptidase. *PLoS ONE*, **2013**, 8, e74518	3.7	11
99	Carboxylated Graphene for Radical-Assisted Ultra-Trace-Level Water Treatment and Noble Metal Recovery. *ACS Nano*, **2021**, 15, 3349-3358	16.7	11
98	Interaction of the Helium, Hydrogen, Air, Argon, and Nitrogen Bubbles with Graphite Surface in Water. *ACS Applied Materials & Interfaces*, **2017**, 9, 17517-17525	9.5	10
97	Flow induced HeLa cell detachment kinetics show that oxygen-containing functional groups in graphene oxide are potent cell adhesion enhancers. *Nanoscale*, **2019**, 11, 3222-3228	7.7	10
96	RNA nanopatterning on graphene. *2D Materials*, **2018**, 5, 031006	5.9	10
95	Microwave Energy Drives "On-Off-On" Spin-Switch Behavior in Nitrogen-Doped Graphene. *Advanced Materials*, **2019**, 31, e1902587	24	10
94	Changes in electrostatic surface potential of Na+/K+-ATPase cytoplasmic headpiece induced by cytoplasmic ligand(s) binding. *Biophysical Journal*, **2009**, 97, 1756-64	2.9	10
93	Regulatory phosphorylation of cyclin-dependent kinase 2: insights from molecular dynamics simulations. *Journal of Molecular Modeling*, **2008**, 14, 761-8	2	10
92	Emerging MXene@Metal-Organic Framework Hybrids: Design Strategies toward Versatile Applications. *ACS Nano*, **2021**,	16.7	10
91	Mechanistic Insight into the Limiting Factors of Graphene-Based Environmental Sensors. *ACS Applied Materials & Interfaces*, **2020**, 12, 39764-39771	9.5	10
90	Transparent and Low-Loss Luminescent Solar Concentrators Based on Self-Trapped Exciton Emission in Lead-Free Double Perovskite Nanocrystals. *ACS Applied Energy Materials*, **2021**, 4, 6445-6453	6.1	10
89	Thermally reduced fluorographenes as efficient electrode materials for supercapacitors. *Nanoscale*, **2019**, 11, 21364-21375	7.7	10
88	Zigzag sp Carbon Chains Passing through an sp Framework: A Driving Force toward Room-Temperature Ferromagnetic Graphene. *ACS Nano*, **2018**, 12, 12847-12859	16.7	10

87	Tailoring Electronic and Magnetic Properties of Graphene by Phosphorus Doping. *ACS Applied Materials & Interfaces*, **2020**, 12, 34074-34085	9.5	9
86	One-Step Synthesis of Janus Fluorographene Derivatives. *Chemistry - A European Journal*, **2020**, 26, 6518-6524	4.8	9
85	How the stabilization of INK4 tumor suppressor 3D structure evaluated by quantum chemical and molecular mechanics calculations corresponds well with experimental results: interplay of association enthalpy, entropy, and solvation effects. *Journal of Physical Chemistry B*, **2006**, 110, 4423-9	3.4	9
84	Rational Design of Graphene Derivatives for Electrochemical Reduction of Nitrogen to Ammonia. *ACS Nano*, **2021**,	16.7	9
83	Anchoring of single-platinum-adatoms on cyanographene: Experiment and theory. *Applied Materials Today*, **2020**, 18, 100462	6.6	9
82	UUCG RNA Tetraloop as a Formidable Force-Field Challenge for MD Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7601-7617	6.4	9
81	Molecular Fluorophores Self-Organize into C-Dot Seeds and Incorporate into C-Dot Structures. *Journal of Physical Chemistry Letters*, **2020**, 11, 8252-8258	6.4	9
80	Dimerization of quercetin, Diels-Alder vs. radical-coupling approach: a joint thermodynamics, kinetics, and topological study. *Journal of Molecular Modeling*, **2016**, 22, 190	2	9
79	First-principles study of the mechanism of wettability transition of defective graphene. *Nanotechnology*, **2017**, 28, 064003	3.4	8
78	Lipocarbazole, an efficient lipid peroxidation inhibitor anchored in the membrane. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 4866-4870	3.4	8
77	Chemical feasibility of the general acid/base mechanism of glmS ribozyme self-cleavage. *Biopolymers*, **2015**, 103, 550-62	2.2	8
76	Tunable one-step double functionalization of graphene based on fluorographene chemistry. *Chemical Communications*, **2020**, 56, 1936-1939	5.8	8
75	The nature of bonding and electronic properties of graphene and benzene with iridium adatoms. *Physical Chemistry Chemical Physics*, **2014**, 16, 20818-27	3.6	8
74	Surface energy analysis (SEA) study of hyaluronan powders. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2013**, 436, 1170-1174	5.1	8
73	Large Enhancement of the Nonlinear Optical Response of Fluorographene by Chemical Functionalization: The Case of Diethyl-amino-fluorographene. *Journal of Physical Chemistry C*, **2019**, 123, 25856-25862	3.8	7
72	Stability of Two-Quartet G-Quadruplexes and Their Dimers in Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 3447-3463	6.4	7
71	Exponential repulsion improves structural predictability of molecular docking. *Journal of Computational Chemistry*, **2016**, 37, 2485-94	3.5	7
70	Pinning ultrasmall greigite nanoparticles on graphene for effective transition-metal-sulfide supercapacitors in an ionic liquid electrolyte. *Journal of Materials Chemistry A*, **2020**, 8, 25716-25726	13	7

69	New Limits for Stability of Supercapacitor Electrode Material Based on Graphene Derivative. *Nanomaterials*, **2020**, 10,	5.4	7
68	Bimodal role of fluorine atoms in fluorographene chemistry opens a simple way toward double functionalization of graphene. *Carbon*, **2019**, 145, 251-258	10.4	6
67	Tuning the magnetic properties of graphene derivatives by functional group selection. *Physical Chemistry Chemical Physics*, **2019**, 21, 12697-12703	3.6	6
66	Metal-organic framework/conductive polymer hybrid materials for supercapacitors. *Applied Materials Today*, **2022**, 26, 101387	6.6	6
65	Covalently Interlinked Graphene Sheets with Sulfur-Chains Enable Superior Lithium–Sulfur Battery Cathodes at Full-Mass Level. *Advanced Functional Materials*, **2021**, 31, 2101326	15.6	6
64	Contribution of the Molecular Fluorophore IPCA to Excitation-Independent Photoluminescence of Carbon Dots. *Journal of Physical Chemistry C*, **2021**, 125, 12140-12148	3.8	6
63	W-RESP: Well-Restrained Electrostatic Potential-Derived Charges. Revisiting the Charge Derivation Model. *Journal of Chemical Theory and Computation*, **2021**, 17, 3495-3509	6.4	6
62	Formic Acid, a Ubiquitous but Overlooked Component of the Early Earth Atmosphere. *Chemistry - A European Journal*, **2020**, 26, 12075-12080	4.8	6
61	Enhanced On-Site Hydrogen Peroxide Electrosynthesis by a Selectively Carboxylated N-Doped Graphene Catalyst. *ChemCatChem*,	5.2	6
60	Graphene Acid for Lithium-Ion Batteries: Carboxylation Boosts Storage Capacity in Graphene. *Advanced Energy Materials*, **2022**, 12, 2103010	21.8	6
59	Single-Atom Catalysis: Mixed-Valence Single-Atom Catalyst Derived from Functionalized Graphene (Adv. Mater. 17/2019). *Advanced Materials*, **2019**, 31, 1970125	24	5
58	Oxidation of metallic two-dimensional transition metal dichalcogenides: 1T-MoS2 and 1T-TaS2. *2D Materials*, **2020**, 7, 045005	5.9	5
57	Two C-terminal ankyrin repeats form the minimal stable unit of the ankyrin repeat protein p18INK4c. *Journal of Molecular Modeling*, **2008**, 14, 747-59	2	5
56	Role of Ionizable Lipids in SARS-CoV-2 Vaccines As Revealed by Molecular Dynamics Simulations: From Membrane Structure to Interaction with mRNA Fragments. *Journal of Physical Chemistry Letters*, **2021**, 12, 11199-11205	6.4	5
55	Hierarchical Porous Graphene-Iron Carbide Hybrid Derived From Functionalized Graphene-Based Metal-Organic Gel as Efficient Electrochemical Dopamine Sensor. *Frontiers in Chemistry*, **2020**, 8, 544	5	5
54	Large magnetic anisotropy in an OsIr dimer anchored in defective graphene. *Nanotechnology*, **2021**, 32,	3.4	5
53	2D graphene derivatives as heterogeneous catalysts to produce biofuels via esterification and trans-esterification reactions. *Applied Materials Today*, **2021**, 23, 101053	6.6	5
52	Multiresponsive 2D TiCT MXene Implanting Molecular Properties. *ACS Nano*, **2021**, 15, 10067-10075	16.7	5

51	Ferromagnetism: Sulfur Doping Induces Strong Ferromagnetic Ordering in Graphene: Effect of Concentration and Substitution Mechanism (Adv. Mater. 25/2016). *Advanced Materials*, **2016**, 28, 5139	24	5
50	Anchoring of Transition Metals to Graphene Derivatives as an Efficient Approach for Designing Single-Atom Catalysts. *Advanced Materials Interfaces*, **2021**, 8, 2001392	4.6	5
49	Graphene with Covalently Grafted Amino Acid as a Route Toward Eco-Friendly and Sustainable Supercapacitors. *ChemSusChem*, **2021**, 14, 3904-3914	8.3	5
48	Label-free and reagentless electrochemical genosensor based on graphene acid for meat adulteration detection. *Biosensors and Bioelectronics*, **2022**, 195, 113628	11.8	5
47	A multifunctional covalently linked graphene–MOF hybrid as an effective chemiresistive gas sensor. *Journal of Materials Chemistry A*, **2021**, 9, 17434-17441	13	5
46	Carbon Nanotube Based Metal-Organic Framework Hybrids From Fundamentals Toward Applications. *Small*, **2021**, e2104628	11	5
45	Graphene: Thiofluorographene—Hydrophilic Graphene Derivative with Semiconducting and Genosensing Properties (Adv. Mater. 14/2015). *Advanced Materials*, **2015**, 27, 2407-2407	24	4
44	Surface Energy of Black Phosphorus Alloys with Arsenic. *ChemNanoMat*, **2020**, 6, 821-826	3.5	4
43	Thermally induced intra-molecular transformation and metalation of free-base porphyrin on Au(111) surface steered by surface confinement and ad-atoms. *Nanoscale Advances*, **2020**, 2, 2986-2991	5.1	4
42	Mapping the Chemical Space of the RNA Cleavage and Its Implications for Ribozyme Catalysis. *Journal of Physical Chemistry B*, **2017**, 121, 10828-10840	3.4	4
41	Ligand effects on single-electron transfer of isolated iron atoms in the gaseous complexes [(OC)mFe(OH2)n]+ (m, n=0–2, m+n=1, 2). *International Journal of Mass Spectrometry*, **2012**, 330-332, 95-99	1.9	4
40	Nitrogen doped graphene with diamond-like bonds achieves unprecedented energy density at high power in a symmetric sustainable supercapacitor.. *Energy and Environmental Science*, **2022**, 15, 740-748	35.4	4
39	Rhenium Doping of Layered Transition-Metal Diselenides Triggers Enhancement of Photoelectrochemical Activity. *ACS Nano*, **2021**, 15, 2374-2385	16.7	4
38	Insights into G-Quadruplex-Hemin Dynamics Using Atomistic Simulations: Implications for Reactivity and Folding. *Journal of Chemical Theory and Computation*, **2021**, 17, 1883-1899	6.4	4
37	Toward Convergence in Folding Simulations of RNA Tetraloops: Comparison of Enhanced Sampling Techniques and Effects of Force Field Modifications.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	4
36	Wobble pairs of the HDV ribozyme play specific roles in stabilization of active site dynamics. *Physical Chemistry Chemical Physics*, **2015**, 17, 5887-900	3.6	3
35	Morphology-Dependent Magnetism in Nanographene: Beyond Nanoribbons. *Advanced Functional Materials*, **2018**, 28, 1800592	15.6	3
34	Hierarchical porous metal–organic framework materials for efficient oil–water separation. *Journal of Materials Chemistry A*, **2022**, 10, 2751-2785	13	3

33	Tuning the UV spectrum of PAHs by means of different N-doping types taking pyrene as paradigmatic example: categorization valence bond theory and high-level computational approaches. *Physical Chemistry Chemical Physics*, **2020**, 22, 22003-22015	3.6	3
32	Surface termination of MgB unveiled by a combination of adsorption experiments and theoretical calculations. *Physical Chemistry Chemical Physics*, **2019**, 21, 7313-7320	3.6	2
31	Carbon-Based Materials at Nanoscale. *Journal of Nanomaterials*, **2015**, 2015, 1-2	3.2	2
30	Fluorographene: Dichlorocarbene-Functionalized Fluorographene: Synthesis and Reaction Mechanism (Small 31/2015). *Small*, **2015**, 11, 3789-3789	11	2
29	The synthesis of some polycyclic N-H acids with quinoxaline and [1,2,4]triazines. *Arkivoc*, **2004**, 2003, 65-74	0.9	2
28	Octylamine-Modified Fluorographenes as a Versatile Platform for the Efficient Engineering of the Nonlinear Optical Properties of Fluorinated Graphenes. *Advanced Photonics Research*, **2020**, 1, 2000014	1.9	2
27	Ultrafine TiO2 Nanoparticle Supported Nitrogen-Rich Graphitic Porous Carbon as an Efficient Anode Material for Potassium-Ion Batteries. *Advanced Energy and Sustainability Research*, **2021**, 2, 2100042	1.6	2
26	Structural Bioinformatics Tools for Drug Design. *SpringerBriefs in Biochemistry and Molecular Biology*, **2016**,		2
25	Band-Edge Engineering at the Carbon Dot□TiO2 Interface by Substitutional Boron Doping. *Journal of Physical Chemistry C*, **2019**, 123, 5980-5988	3.8	2
24	Two-dimensional MOF-based liquid marbles: surface energy calculations and efficient oil□water separation using a ZIF-9-III@PVDF membrane. *Journal of Materials Chemistry A*,	13	2
23	Recent advancements in metal□organic frameworks integrating quantum dots (QDs@MOF) and their potential applications. *Nanotechnology Reviews*, **2022**, 11, 1947-1976	6.3	2
22	Atomic-Scale Edge Morphology, Stability, and Oxidation of Single-Layer 2H-TaS. *ChemPlusChem*, **2020**, 85, 2557-2564	2.8	1
21	Insenstivity to close contacts and inability to predict protein foldability. *Journal of Biomolecular Structure and Dynamics*, **2011**, 28, 633-4; discussion 669-674	3.6	1
20	Graphene Lattices with Embedded Transition-Metal Atoms and Tunable Magnetic Anisotropy Energy: Implications for Spintronic Devices. *ACS Applied Nano Materials*, **2022**, 5, 1562-1573	5.6	1
19	W-RESP: Well-Restrained Electrostatic Potential Derived Charges. Revisiting the Charge Derivation Model		1
18	Stability of Two-quartet G-quadruplexes and Their Dimers in Atomistic Simulations		1
17	Improving The Performance Of The Amber Rna Force Field By Tuning The Hydrogen-Bonding Interactions		1
16	Stretch-Healable Molecular Nanofibers. *Advanced Theory and Simulations*, **2020**, 3, 2000094	3.5	1

15	Detection of Channels. *SpringerBriefs in Biochemistry and Molecular Biology*, **2016**, 59-69		1
14	On-Surface Synthesis of One-Dimensional Coordination Polymers with Tailored Magnetic Anisotropy. *ACS Applied Materials & Interfaces*, **2021**, 13, 32393-32401	9.5	1
13	Flax-Derived Carbon: A Highly Durable Electrode Material for Electrochemical Double-Layer Supercapacitors. *Nanomaterials*, **2021**, 11,	5.4	1
12	Molecular insights from theoretical calculations explain the differences in affinity and diffusion of airborne contaminants on surfaces of hBN and graphene. *Applied Surface Science*, **2021**, 565, 150382	6.7	1
11	Unveiling the true band gap of fluorographene and its origins by teaming theory and experiment. *Applied Surface Science*, **2022**, 587, 152839	6.7	1
10	Graphene Field Effect Transistors: A Sensitive Platform for Detecting Sarin.. *ACS Applied Materials & Interfaces*, **2021**, 13, 61751-61757	9.5	1
9	Accessibility of Grafted Functional Groups Limits Reactivity of Covalent Graphene Derivatives. *Applied Surface Science*, **2022**, 153792	6.7	1
8	Lipid bilayer position and orientation of novel carprofens, modulators of -secretase in Alzheimer's disease. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 2224-2233	3.8	0
7	Controlled nucleation of crystallization process as an efficient tool to tune the properties of corticosteroid API. *Powder Technology*, **2022**, 117334	5.2	0
6	Graphene: High-Performance Supercapacitors Based on a Zwitterionic Network of Covalently Functionalized Graphene with Iron Tetraaminophthalocyanine (Adv. Funct. Mater. 29/2018). *Advanced Functional Materials*, **2018**, 28, 1870203	15.6	
5	Graphene: Morphology-Dependent Magnetism in Nanographene: Beyond Nanoribbons (Adv. Funct. Mater. 22/2018). *Advanced Functional Materials*, **2018**, 28, 1870147	15.6	
4	Structure-Function Relationships Within the Hepatitis Delta Virus Ribozyme. *Biophysical Journal*, **2012**, 102, 277a	2.9	
3	Structural Bioinformatics Databases of General Use. *SpringerBriefs in Biochemistry and Molecular Biology*, **2016**, 17-30		
2	Structural properties of CYP2D6: requirements for substrates and inhibitors **2014**, 68-78		
1	Biomacromolecular Fragments and Patterns. *SpringerBriefs in Biochemistry and Molecular Biology*, **2016**, 7-15		