Michal Otyepka

List of Publications by Year in Descending Order

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	Hierarchical porous metal–organic framework materials for efficient oil–water separation. *Journal of Materials Chemistry A*, **2022**, 10, 2751-2785	13	3
319	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
318	Metal-organic framework/conductive polymer hybrid materials for supercapacitors. *Applied Materials Today*, **2022**, 26, 101387	6.6	6
317	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
316	Label-free and reagentless electrochemical genosensor based on graphene acid for meat adulteration detection. *Biosensors and Bioelectronics*, **2022**, 195, 113628	11.8	5
315	Controlled nucleation of crystallization process as an efficient tool to tune the properties of corticosteroid API. *Powder Technology*, **2022**, 117334	5.2	0
314	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
313	Unveiling the true band gap of fluorographene and its origins by teaming theory and experiment. *Applied Surface Science*, **2022**, 587, 152839	6.7	1
312	Graphene Acid for Lithium-Ion Batteries: Carboxylation Boosts Storage Capacity in Graphene. *Advanced Energy Materials*, **2022**, 12, 2103010	21.8	6
311	Recent advancements in metal–organic frameworks integrating quantum dots (QDs@MOF) and their potential applications. *Nanotechnology Reviews*, **2022**, 11, 1947-1976	6.3	2
310	Accessibility of Grafted Functional Groups Limits Reactivity of Covalent Graphene Derivatives. *Applied Surface Science*, **2022**, 153792	6.7	1
309	Emerging MXene@Metal-Organic Framework Hybrids: Design Strategies toward Versatile Applications. *ACS Nano*, **2021**,	16.7	10
308	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
307	Rational Design of Graphene Derivatives for Electrochemical Reduction of Nitrogen to Ammonia. *ACS Nano*, **2021**,	16.7	9
306	Single Co-Atoms as Electrocatalysts for Efficient Hydrazine Oxidation Reaction. *Small*, **2021**, 17, e2006477	11	16
305	Large magnetic anisotropy in an OsIr dimer anchored in defective graphene. *Nanotechnology*, **2021**, 32,	3.4	5
304	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. *Applied Materials Today*, **2021**, 22, 100924	6.6	23

303	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
302	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
301	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
300	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
299	Silver Covalently Bound to Cyanographene Overcomes Bacterial Resistance to Silver Nanoparticles and Antibiotics. *Advanced Science*, **2021**, 8, 2003090	13.6	13
298	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
297	2D graphene derivatives as heterogeneous catalysts to produce biofuels via esterification and trans-esterification reactions. *Applied Materials Today*, **2021**, 23, 101053	6.6	5
296	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
295	Multiresponsive 2D TiCT MXene Implanting Molecular Properties. *ACS Nano*, **2021**, 15, 10067-10075	16.7	5
294	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
293	Covalent Graphene-MOF Hybrids for High-Performance Asymmetric Supercapacitors. *Advanced Materials*, **2021**, 33, e2004560	24	51
292	Carboxylated Graphene for Radical-Assisted Ultra-Trace-Level Water Treatment and Noble Metal Recovery. *ACS Nano*, **2021**, 15, 3349-3358	16.7	11
291	Rhenium Doping of Layered Transition-Metal Diselenides Triggers Enhancement of Photoelectrochemical Activity. *ACS Nano*, **2021**, 15, 2374-2385	16.7	4
290	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
289	On-Surface Synthesis of One-Dimensional Coordination Polymers with Tailored Magnetic Anisotropy. *ACS Applied Materials & Interfaces*, **2021**, 13, 32393-32401	9.5	1
288	Flax-Derived Carbon: A Highly Durable Electrode Material for Electrochemical Double-Layer Supercapacitors. *Nanomaterials*, **2021**, 11,	5.4	1
287	Recent Progress in Emerging Two-Dimensional Transition Metal Carbides. *Nano-Micro Letters*, **2021**, 13, 183	19.5	24
286	Graphene with Covalently Grafted Amino Acid as a Route Toward Eco-Friendly and Sustainable Supercapacitors. *ChemSusChem*, **2021**, 14, 3904-3914	8.3	5

285	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
284	A multifunctional covalently linked graphene/MOF hybrid as an effective chemiresistive gas sensor. *Journal of Materials Chemistry A*, **2021**, 9, 17434-17441	13	5
283	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
282	Graphene Field Effect Transistors: A Sensitive Platform for Detecting Sarin.. *ACS Applied Materials & Interfaces*, **2021**, 13, 61751-61757	9.5	1
281	Carbon Nanotube Based Metal-Organic Framework Hybrids From Fundamentals Toward Applications. *Small*, **2021**, e2104628	11	5
280	Atomic-Scale Edge Morphology, Stability, and Oxidation of Single-Layer 2H-TaS. *ChemPlusChem*, **2020**, 85, 2557-2564	2.8	1
279	Surface Energy of Black Phosphorus Alloys with Arsenic. *ChemNanoMat*, **2020**, 6, 821-826	3.5	4
278	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
277	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
276	Oxidation of metallic two-dimensional transition metal dichalcogenides: 1T-MoS2 and 1T-TaS2. *2D Materials*, **2020**, 7, 045005	5.9	5
275	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
274	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
273	Tailoring Electronic and Magnetic Properties of Graphene by Phosphorus Doping. *ACS Applied Materials & Interfaces*, **2020**, 12, 34074-34085	9.5	9
272	One-Step Synthesis of Janus Fluorographene Derivatives. *Chemistry - A European Journal*, **2020**, 26, 6518-6524	4.8	9
271	Tunable Synthesis of Nitrogen Doped Graphene from Fluorographene under Mild Conditions. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 4764-4772	8.3	17
270	Tunable one-step double functionalization of graphene based on fluorographene chemistry. *Chemical Communications*, **2020**, 56, 1936-1939	5.8	8
269	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
268	Anchoring of single-platinum-adatoms on cyanographene: Experiment and theory. *Applied Materials Today*, **2020**, 18, 100462	6.6	9

267	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
266	Immobilized Enzymes on Graphene as Nanobiocatalyst. *ACS Applied Materials & Interfaces*, **2020**, 12, 250-259	9.5	29
265	Unique cellular network formation guided by heterostructures based on reduced graphene oxide - TiCT MXene hydrogels. *Acta Biomaterialia*, **2020**, 115, 104-115	10.8	15
264	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
263	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
262	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
261	Mechanistic Insight into the Limiting Factors of Graphene-Based Environmental Sensors. *ACS Applied Materials & Interfaces*, **2020**, 12, 39764-39771	9.5	10
260	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
259	Human virus detection with graphene-based materials. *Biosensors and Bioelectronics*, **2020**, 166, 112436	11.8	74
258	Metal Halide Perovskite@Metal-Organic Framework Hybrids: Synthesis, Design, Properties, and Applications. *Small*, **2020**, 16, e2004891	11	16
257	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
256	New Limits for Stability of Supercapacitor Electrode Material Based on Graphene Derivative. *Nanomaterials*, **2020**, 10,	5.4	7
255	Tailoring □conjugation and vibrational modes to steer on-surface synthesis of pentalene-bridged ladder polymers. *Nature Communications*, **2020**, 11, 4567	17.4	12
254	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
253	Stretch-Healable Molecular Nanofibers. *Advanced Theory and Simulations*, **2020**, 3, 2000094	3.5	1
252	Formic Acid, a Ubiquitous but Overlooked Component of the Early Earth Atmosphere. *Chemistry - A European Journal*, **2020**, 26, 12075-12080	4.8	6
251	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
250	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

249	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
248	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
247	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
246	Alkynylation of graphene via the Sonogashira C-C cross-coupling reaction on fluorographene. *Chemical Communications*, **2019**, 55, 1088-1091	5.8	15
245	Tuning the magnetic properties of graphene derivatives by functional group selection. *Physical Chemistry Chemical Physics*, **2019**, 21, 12697-12703	3.6	6
244	Chemical Tuning of Specific Capacitance in Functionalized Fluorographene. *Chemistry of Materials*, **2019**, 31, 4698-4709	9.6	19
243	Hydrophobic Metal-Organic Frameworks. *Advanced Materials*, **2019**, 31, e1900820	24	76
242	Single-Atom Catalysis: Mixed-Valence Single-Atom Catalyst Derived from Functionalized Graphene (Adv. Mater. 17/2019). *Advanced Materials*, **2019**, 31, 1970125	24	5
241	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
240	Ion Interactions across Graphene in Electrolyte Aqueous Solutions. *Journal of Physical Chemistry C*, **2019**, 123, 9799-9806	3.8	14
239	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
238	Thiophenol-Modified Fluorographene Derivatives for Nonlinear Optical Applications. *ChemPlusChem*, **2019**, 84, 1288-1298	2.8	11
237	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
236	Mixed-Valence Single-Atom Catalyst Derived from Functionalized Graphene. *Advanced Materials*, **2019**, 31, e1900323	24	76
235	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
234	Intrinsic photoluminescence of amine-functionalized graphene derivatives for bioimaging applications. *Applied Materials Today*, **2019**, 17, 112-122	6.6	17
233	Microwave Energy Drives "On-Off-On" Spin-Switch Behavior in Nitrogen-Doped Graphene. *Advanced Materials*, **2019**, 31, e1902587	24	10
232	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

231	Shape-Assisted 2D MOF/Graphene Derived Hybrids as Exceptional Lithium-Ion Battery Electrodes. *Advanced Functional Materials*, **2019**, 29, 1902539	15.6	71
230	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
229	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
228	Selective Functionalization Blended with Scaffold Conductivity in Graphene Acid Promotes HO Electrochemical Sensing. *ACS Omega*, **2019**, 4, 19944-19952	3.9	12
227	Thermally reduced fluorographenes as efficient electrode materials for supercapacitors. *Nanoscale*, **2019**, 11, 21364-21375	7.7	10
226	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
225	Covalently functionalized graphene as a supercapacitor electrode material. *FlatChem*, **2019**, 13, 25-33	5.1	42
224	Arene CH insertion catalyzed by ferrocene covalently heterogenized on graphene acid. *Carbon*, **2019**, 143, 318-328	10.4	17
223	Membrane-attached mammalian cytochromes P450: An overview of the membrane effects on structure, drug binding, and interactions with redox partners. *Journal of Inorganic Biochemistry*, **2018**, 183, 117-136	4.2	64
222	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
221	Role of the puckered anisotropic surface in the surface and adsorption properties of black phosphorus. *Nanoscale*, **2018**, 10, 8979-8988	7.7	23
220	Morphology-Dependent Magnetism in Nanographene: Beyond Nanoribbons. *Advanced Functional Materials*, **2018**, 28, 1800592	15.6	3
219	Reactivity of fluorographene is triggered by point defects: beyond the perfect 2D world. *Nanoscale*, **2018**, 10, 4696-4707	7.7	45
218	ChannelsDB: database of biomacromolecular tunnels and pores. *Nucleic Acids Research*, **2018**, 46, D399-D405	20.2	22
217	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. *Chemical Reviews*, **2018**, 118, 4177-4338	68.1	235
216	RNA nanopatterning on graphene. *2D Materials*, **2018**, 5, 031006	5.9	10
215	Structural patterns of the human ABCC4/MRP4 exporter in lipid bilayers rationalize clinically observed polymorphisms. *Pharmacological Research*, **2018**, 133, 318-327	10.2	11
214	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	

213	Non-covalent control of spin-state in metal-organic complex by positioning on N-doped graphene. *Nature Communications*, **2018**, 9, 2831	17.4	52
212	Graphene: Morphology-Dependent Magnetism in Nanographene: Beyond Nanoribbons (Adv. Funct. Mater. 22/2018). *Advanced Functional Materials*, **2018**, 28, 1870147	15.6	
211	2D Chemistry: Chemical Control of Graphene Derivatization. *Journal of Physical Chemistry Letters*, **2018**, 9, 3580-3585	6.4	34
210	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
209	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
208	Bonding Motifs in Metal-Organic Compounds on Surfaces. *Journal of the American Chemical Society*, **2018**, 140, 12884-12889	16.4	13
207	Lipid bilayer position and orientation of novel carprofens, modulators of β-secretase in Alzheimer's disease. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 2224-2233	3.8	0
206	Structural dynamics of propeller loop: towards folding of RNA G-quadruplex. *Nucleic Acids Research* , **2018**, 46, 8754-8771	20.1	18
205	MOLEonline: a web-based tool for analyzing channels, tunnels and pores (2018 update). *Nucleic Acids Research*, **2018**, 46, W368-W373	20.1	112
204	High-Performance Supercapacitors Based on a Zwitterionic Network of Covalently Functionalized Graphene with Iron Tetraaminophthalocyanine. *Advanced Functional Materials*, **2018**, 28, 1801111	15.6	32
203	Role of the Edge Properties in the Hydrogen Evolution Reaction on MoS. *Chemistry - A European Journal*, **2017**, 23, 4863-4869	4.8	27
202	Doping with Graphitic Nitrogen Triggers Ferromagnetism in Graphene. *Journal of the American Chemical Society*, **2017**, 139, 3171-3180	16.4	124
201	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
200	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
199	High-Yield Alkylation and Arylation of Graphene via Grignard Reaction with Fluorographene. *Chemistry of Materials*, **2017**, 29, 926-930	9.6	55
198	Functional Nanosheet Synthons by Covalent Modification of Transition-Metal Dichalcogenides. *Chemistry of Materials*, **2017**, 29, 2066-2073	9.6	38
197	Room temperature organic magnets derived from sp functionalized graphene. *Nature Communications*, **2017**, 8, 14525	17.4	81
196	Cyanographene and Graphene Acid: Emerging Derivatives Enabling High-Yield and Selective Functionalization of Graphene. *ACS Nano*, **2017**, 11, 2982-2991	16.7	99

195	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
194	Nonenzymatic Oligomerization of 3′,5′-Cyclic CMP Induced by Proton and UV Irradiation Hints at a Nonfastidious Origin of RNA. *ChemBioChem*, **2017**, 18, 1535-1543	3.8	12
193	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
192	Chemistry, properties, and applications of fluorographene. *Applied Materials Today*, **2017**, 9, 60-70	6.6	154
191	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
190	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
189	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
188	First-principles study of the mechanism of wettability transition of defective graphene. *Nanotechnology*, **2017**, 28, 064003	3.4	8
187	Is Single Layer MoS Stable in the Air?. *Chemistry - A European Journal*, **2017**, 23, 13233-13239	4.8	57
186	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
185	Graphitic Nitrogen Triggers Red Fluorescence in Carbon Dots. *ACS Nano*, **2017**, 11, 12402-12410	16.7	351
184	Surface properties of MoS probed by inverse gas chromatography and their impact on electrocatalytic properties. *Nanoscale*, **2017**, 9, 19236-19244	7.7	15
183	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
182	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
181	How to understand atomistic molecular dynamics simulations of RNA and protein-RNA complexes?. *Wiley Interdisciplinary Reviews RNA*, **2017**, 8, e1405	9.3	42
180	Direct mapping of chemical oxidation of individual graphene sheets through dynamic force measurements at the nanoscale. *Nanoscale*, **2017**, 9, 119-127	7.7	17
179	Modelling of graphene functionalization. *Physical Chemistry Chemical Physics*, **2016**, 18, 6351-72	3.6	161
178	Exponential repulsion improves structural predictability of molecular docking. *Journal of Computational Chemistry*, **2016**, 37, 2485-94	3.5	7

177	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. *Journal of Chemical Theory and Computation*, **2016**, 12, 4534-48	6.4	77
176	Organic adsorbates have higher affinities to fluorographene than to graphene. *Applied Materials Today*, **2016**, 5, 142-149	6.6	39
175	Assessing the Current State of Amber Force Field Modifications for DNA. *Journal of Chemical Theory and Computation*, **2016**, 12, 4114-27	6.4	203
174	The Role of Protein-Protein and Protein-Membrane Interactions on P450 Function. *Drug Metabolism and Disposition*, **2016**, 44, 576-90	4	27
173	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
172	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
171	Stabilizing and Modulating Color by Copigmentation: Insights from Theory and Experiment. *Chemical Reviews*, **2016**, 116, 4937-82	68.1	258
170	Graphitic Nitrogen Doping in Carbon Dots Causes Red-Shifted Absorption. *Journal of Physical Chemistry C*, **2016**, 120, 1303-1308	3.8	149
169	Structural Bioinformatics Databases of General Use. *SpringerBriefs in Biochemistry and Molecular Biology*, **2016**, 17-30		
168	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
167	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
166	In silico pharmacology: Drug membrane partitioning and crossing. *Pharmacological Research*, **2016**, 111, 471-486	10.2	33
165	Sulfur Doping Induces Strong Ferromagnetic Ordering in Graphene: Effect of Concentration and Substitution Mechanism. *Advanced Materials*, **2016**, 28, 5045-53	24	67
164	Biomimetische superhydrophobe/superoleophile hoch fluorierte Graphenoxid-ZIF-8-Komposite f□ die □Wasser-Trennung. *Angewandte Chemie*, **2016**, 128, 1193-1197	3.6	12
163	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
162	Structural Bioinformatics Tools for Drug Design. *SpringerBriefs in Biochemistry and Molecular Biology*, **2016**,		2
161	Biomacromolecular Fragments and Patterns. *SpringerBriefs in Biochemistry and Molecular Biology*, **2016**, 7-15		
160	Detection of Channels. *SpringerBriefs in Biochemistry and Molecular Biology*, **2016**, 59-69		1

159	Photoluminescent Carbon Nanostructures. *Chemistry of Materials*, **2016**, 28, 4085-4128	9.6	150
158	Effect of Lipid Charge on Membrane Immersion of Cytochrome P450 3A4. *Journal of Physical Chemistry B*, **2016**, 120, 11205-11213	3.4	17
157	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
156	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
155	Thiofluorographene-hydrophilic graphene derivative with semiconducting and genosensing properties. *Advanced Materials*, **2015**, 27, 2305-10	24	74
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