Michal Otyepka

List of Publications by Year
in descending order

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324 papers	23,434 citations	9786 73 h-index	10734 138 g-index
341 all docs	341 docs citations	341 times ranked	26335 citing authors

#	Article	IF	Citations
1	Functionalization of Graphene: Covalent and Non-Covalent Approaches, Derivatives and Applications. Chemical Reviews, 2012, 112, 6156-6214.	47.7	3,531
2	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.	5.3	873
3	Graphitic Nitrogen Triggers Red Fluorescence in Carbon Dots. ACS Nano, 2017, 11, 12402-12410.	14.6	550
4	CAVER: a new tool to explore routes from protein clefts, pockets and cavities. BMC Bioinformatics, 2006, 7, 316.	2.6	453
5	Stabilizing and Modulating Color by Copigmentation: Insights from Theory and Experiment. Chemical Reviews, 2016, 116, 4937-4982.	47.7	408
6	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. Chemical Reviews, 2018, 118, 4177-4338.	47.7	408
7	Adsorption of Small Organic Molecules on Graphene. Journal of the American Chemical Society, 2013, 135, 6372-6377.	13.7	407
8	Refinement of the Sugarâ€“Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. Journal of Chemical Theory and Computation, 2015, 11, 5723-5736.	5.3	392
9	Graphene Fluoride: A Stable Stoichiometric Graphene Derivative and its Chemical Conversion to Graphene. Small, 2010, 6, 2885-2891.	10.0	386
10	Biomimetic Superhydrophobic/Superoleophilic Highly Fluorinated Graphene Oxide and ZIFâ€8 Composites for Oilâ€“Water Separation. Angewandte Chemie - International Edition, 2016, 55, 1178-1182.	13.8	370
11	Assessing the Current State of Amber Force Field Modifications for DNA. Journal of Chemical Theory and Computation, 2016, 12, 4114-4127.	5.3	351
12	Halogenated Graphenes: Rapidly Growing Family of Graphene Derivatives. ACS Nano, 2013, 7, 6434-6464.	14.6	349
13	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.	5.3	339
14	MOLE 2.0: advanced approach for analysis of biomacromolecular channels. Journal of Cheminformatics, 2013, 5, 39.	6.1	262
15	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. Journal of Chemical Theory and Computation, 2013, 9, 2339-2354.	5.3	255
16	Photoluminescence effects of graphitic core size and surface functional groups in carbon dots: COOâ¯ induced red-shift emission. Carbon, 2014, 70, 279-286.	10.3	240
17	Redesigning dehalogenase access tunnels as a strategy for degrading an anthropogenic substrate. Nature Chemical Biology, 2009, 5, 727-733.	8.0	238
18	Reference Simulations of Noncanonical Nucleic Acids with Different Ï‡ Variants of the AMBER Force Field: Quadruplex DNA, Quadruplex RNA, and Z-DNA. Journal of Chemical Theory and Computation, 2012, 8, 2506-2520.	5.3	231

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19	Chemistry, properties, and applications of fluorographene. Applied Materials Today, 2017, 9, 60-70.	4.3	211
20	MOLE: A Voronoi Diagram-Based Explorer of Molecular Channels, Pores, and Tunnels. Structure, 2007, 15, 1357-1363.	3.3	210
21	MOLEonline: a web-based tool for analyzing channels, tunnels and pores (2018 update). Nucleic Acids Research, 2018, 46, W368-W373.	14.5	208
22	Graphitic Nitrogen Doping in Carbon Dots Causes Red-Shifted Absorption. Journal of Physical Chemistry C, 2016, 120, 1303-1308.	3.1	207
23	Doping with Graphitic Nitrogen Triggers Ferromagnetism in Graphene. Journal of the American Chemical Society, 2017, 139, 3171-3180.	13.7	202
24	Modelling of graphene functionalization. Physical Chemistry Chemical Physics, 2016, 18, 6351-6372.	2.8	190
25	Photoluminescent Carbon Nanostructures. Chemistry of Materials, 2016, 28, 4085-4128.	6.7	186
26	Spectroscopic Fingerprints of Graphitic, Pyrrolic, Pyridinic, and Chemisorbed Nitrogen in N-Doped Graphene. Journal of Physical Chemistry C, 2019, 123, 10695-10702.	3.1	181
27	Molecular Dynamics and Quantum Mechanics of RNA: Conformational and Chemical Change We Can Believe In. Accounts of Chemical Research, 2010, 43, 40-47.	15.6	155
28	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, 4155-4164.	5.3	142
29	Human virus detection with graphene-based materials. Biosensors and Bioelectronics, 2020, 166, 112436.	10.1	140
30	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. Journal of Physical Chemistry Letters, 2014, 5, 1771-1782.	4.6	139
31	Hydrophobic Metalâ€“Organic Frameworks. Advanced Materials, 2019, 31, e1900820.	21.0	138
32	Base Pair Fraying in Molecular Dynamics Simulations of DNA and RNA. Journal of Chemical Theory and Computation, 2014, 10, 3177-3189.	5.3	135
33	Cyanographene and Graphene Acid: Emerging Derivatives Enabling High-Yield and Selective Functionalization of Graphene. ACS Nano, 2017, 11, 2982-2991.	14.6	133
34	Mixedâ€Valence Singleâ€Atom Catalyst Derived from Functionalized Graphene. Advanced Materials, 2019, 31, e1900323.	21.0	129
35	Membrane Position of Ibuprofen Agrees with Suggested Access Path Entrance to Cytochrome P450 2C9 Active Site. Journal of Physical Chemistry A, 2011, 115, 11248-11255.	2.5	128
36	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. Journal of Chemical Theory and Computation, 2016, 12, 4534-4548.	5.3	125

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37	MOLEonline 2.0: interactive web-based analysis of biomacromolecular channels. Nucleic Acids Research, 2012, 40, W222-W227.	14.5	123
38	Covalent Grapheneâ€MOF Hybrids for Highâ€Performance Asymmetric Supercapacitors. Advanced Materials, 2021, 33, e2004560.	21.0	121
39	What common structural features and variations of mammalian P450s are known to date?. Biochimica Et Biophysica Acta - General Subjects, 2007, 1770, 376-389.	2.4	119
40	Positioning of Antioxidant Quercetin and Its Metabolites in Lipid Bilayer Membranes: Implication for Their Lipid-Peroxidation Inhibition. Journal of Physical Chemistry B, 2012, 116, 1309-1318.	2.6	119
41	Shapeâ€Assisted 2D MOF/Graphene Derived Hybrids as Exceptional Lithiumâ€Ion Battery Electrodes. Advanced Functional Materials, 2019, 29, 1902539.	14.9	118
42	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.	3.5	117
43	Anaerobic Reaction of Nanoscale Zerovalent Iron with Water: Mechanism and Kinetics. Journal of Physical Chemistry C, 2014, 118, 13817-13825.	3.1	114
44	Room temperature organic magnets derived from sp3 functionalized graphene. Nature Communications, 2017, 8, 14525.	12.8	112
45	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, 8165-8173.	2.6	111
46	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, 3569-3579.	5.3	108
47	Nature and magnitude of aromatic base stacking in DNA and RNA: Quantum chemistry, molecular mechanics, and experiment. Biopolymers, 2013, 99, 978-988.	2.4	106
48	Convergence of Free Energy Profile of Coumarin in Lipid Bilayer. Journal of Chemical Theory and Computation, 2012, 8, 1200-1211.	5.3	102
49	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.	3.0	101
50	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.	5.3	100
51	Environmental Applications of Chemically Pure Natural Ferrihydrite. Environmental Science & Technology, 2007, 41, 4367-4374.	10.0	97
52	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.	5.3	97
53	Nature of Absorption Bands in Oxygen-Functionalized Graphitic Carbon Dots. Journal of Physical Chemistry C, 2015, 119, 13369-13373.	3.1	96
54	Behavior of Human Cytochromes P450 on Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 11556-11564.	2.6	94

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55	Sulfur Doping Induces Strong Ferromagnetic Ordering in Graphene: Effect of Concentration and Substitution Mechanism. Advanced Materials, 2016, 28, 5045-5053.	21.0	94
56	Reactivity of Fluorographene: A Facile Way toward Graphene Derivatives. Journal of Physical Chemistry Letters, 2015, 6, 1430-1434.	4.6	90
57	Anatomy of enzyme channels. BMC Bioinformatics, 2014, 15, 379.	2.6	89
58	Amphiphilic Drug-Like Molecules Accumulate in a Membrane below the Head Group Region. Journal of Physical Chemistry B, 2014, 118, 1030-1039.	2.6	89
59	Folding of guanine quadruplex moleculesâ€“funnel-like mechanism or kinetic partitioning? An overview from MD simulation studies. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 1246-1263.	2.4	89
60	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. Journal of Chemical Theory and Computation, 2013, 9, 4287-4292.	5.3	88
61	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.	10.3	87
62	Chemical nature of boron and nitrogen dopant atoms in graphene strongly influences its electronic properties. Physical Chemistry Chemical Physics, 2014, 16, 14231-14235.	2.8	86
63	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, 1449-1457.	7.6	85
64	Computer Folding of RNA Tetraloops? Are We There Yet?. Journal of Chemical Theory and Computation, 2013, 9, 2115-2125.	5.3	84
65	Thiofluorographeneâ€“Hydrophilic Graphene Derivative with Semiconducting and Genosensing Properties. Advanced Materials, 2015, 27, 2305-2310.	21.0	84
66	Crystal Structure of Haloalkane Dehalogenase LinB from Sphingomonas paucimobilis UT26 at 0.95 Ã... Resolution:â€‰ Dynamics of Catalytic Residues,. Biochemistry, 2004, 43, 870-878.	2.5	82
67	Theoretical studies of RNA catalysis: Hybrid QM/MM methods and their comparison with MD and QM. Methods, 2009, 49, 202-216.	3.8	82
68	Quaternized carbon dot-modified graphene oxide for selective cell labelling â€“ controlled nucleus and cytoplasm imaging. Chemical Communications, 2014, 50, 10782.	4.1	82
69	Recent Progress in Emerging Two-Dimensional Transition Metal Carbides. Nano-Micro Letters, 2021, 13, 183.	27.0	82
70	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, 6642-6652.	2.6	81
71	Emerging MXene@Metalâ€“Organic Framework Hybrids: Design Strategies toward Versatile Applications. ACS Nano, 2021, 15, 18742-18776.	14.6	81
72	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, 8581-8589.	2.6	80

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73	Is Single Layer MoS₂ Stable in the Air?. Chemistry - A European Journal, 2017, 23, 13233-13239.	3.3	80
74	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.	2.8	79
75	The DNA and RNA sugarâ€“phosphate backbone emerges as the key player. An overview of quantum-chemical, structural biology and simulation studies. Physical Chemistry Chemical Physics, 2012, 14, 15257.	2.8	76
76	In SilicoStructural and Functional Analysis of Fragments of the Ankyrin Repeat Protein p18^{INK4c}. Journal of Biomolecular Structure and Dynamics, 2010, 27, 521-539.	3.5	74
77	Quantification of the Interaction Forces between Metals and Graphene by Quantum Chemical Calculations and Dynamic Force Measurements under Ambient Conditions. ACS Nano, 2013, 7, 1646-1651.	14.6	73
78	Benchmarking of Force Fields for Moleculeâ€“Membrane Interactions. Journal of Chemical Theory and Computation, 2014, 10, 4143-4151.	5.3	73
79	Force-Field Dependence of Chignolin Folding and Misfolding: Comparison with Experiment and Redesign. Biophysical Journal, 2012, 102, 1897-1906.	0.5	71
80	Non-covalent control of spin-state in metal-organic complex by positioning on N-doped graphene. Nature Communications, 2018, 9, 2831.	12.8	68
81	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, 2448-2460.	5.3	67
82	Can We Execute Stable Microsecond-Scale Atomistic Simulations of Proteinâ€“RNA Complexes?. Journal of Chemical Theory and Computation, 2015, 11, 1220-1243.	5.3	67
83	Dependence of A-RNA simulations on the choice of the force field and salt strength. Physical Chemistry Chemical Physics, 2009, 11, 10701.	2.8	66
84	Hydrophilic Nanotube Supported Grapheneâ€“Water Dispersible Carbon Superstructure with Excellent Conductivity. Advanced Functional Materials, 2015, 25, 1481-1487.	14.9	66
85	Simulations of A-RNA Duplexes. The Effect of Sequence, Solute Force Field, Water Model, and Salt Concentration. Journal of Physical Chemistry B, 2012, 116, 9899-9916.	2.6	64
86	High-Yield Alkylation and Arylation of Graphene via Grignard Reaction with Fluorographene. Chemistry of Materials, 2017, 29, 926-930.	6.7	64
87	Docking-Based Development of Purine-like Inhibitors of Cyclin-Dependent Kinase-2. Journal of Medicinal Chemistry, 2000, 43, 2506-2513.	6.4	62
88	Synergism of antioxidant action of vitamins E, C and quercetin is related to formation of molecular associations in biomembranes. Chemical Communications, 2015, 51, 7713-7716.	4.1	62
89	Covalently functionalized graphene as a supercapacitor electrode material. FlatChem, 2019, 13, 25-33.	5.6	61
90	Is There a Relationship Between the Substrate Preferences and Structural Flexibility of Cytochromes P450?. Current Drug Metabolism, 2012, 13, 130-142.	1.2	60

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91	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, 3866-3877.	5.3	60
92	Fluorinated graphenes as advanced biosensors â€“ effect of fluorine coverage on electron transfer properties and adsorption of biomolecules. Nanoscale, 2016, 8, 12134-12142.	5.6	60
93	Interaction of single- and double-stranded DNA with multilayer MXene by fluorescence spectroscopy and molecular dynamics simulations. Chemical Science, 2019, 10, 10010-10017.	7.4	59
94	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. Applied Materials Today, 2021, 22, 100924.	4.3	57
95	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, 1608-1622.	5.3	56
96	Functional Nanosheet Synthons by Covalent Modification of Transition-Metal Dichalcogenides. Chemistry of Materials, 2017, 29, 2066-2073.	6.7	56
97	Immobilized Enzymes on Graphene as Nanobiocatalyst. ACS Applied Materials & Interfaces, 2020, 12, 250-259.	8.0	56
98	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.	2.3	55
99	Reactivity of fluorographene is triggered by point defects: beyond the perfect 2D world. Nanoscale, 2018, 10, 4696-4707.	5.6	55
100	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, 8701-8712.	2.6	54
101	How to understand atomistic molecular dynamics simulations of <scp>RNA</scp> and proteinâ€“<scp>RNA</scp> complexes?. Wiley Interdisciplinary Reviews RNA, 2017, 8, e1405.	6.4	54
102	Identification of tunnels in proteins, nucleic acids, inorganic materials and molecular ensembles. Biotechnology Journal, 2007, 2, 62-67.	3.5	53
103	The surface and structural properties of graphite fluoride. Carbon, 2015, 94, 804-809.	10.3	53
104	Water dispersible functionalized graphene fluoride with significant nonlinear optical response. Chemical Physics Letters, 2012, 543, 101-105.	2.6	52
105	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.	30.8	51
106	Molecular Insight into Affinities of Drugs and Their Metabolites to Lipid Bilayers. Journal of Physical Chemistry B, 2013, 117, 2403-2410.	2.6	50
107	In silico pharmacology: Drug membrane partitioning and crossing. Pharmacological Research, 2016, 111, 471-486.	7.1	50
108	Effect of Monovalent Ion Parameters on Molecular Dynamics Simulations of G-Quadruplexes. Journal of Chemical Theory and Computation, 2017, 13, 3911-3926.	5.3	50

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109	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, 2963-2980.	5.3	49
110	Dynamics and Hydration of the Active Sites of Mammalian Cytochromes P450 Probed by Molecular Dynamics Simulations. Current Drug Metabolism, 2012, 13, 177-189.	1.2	49
111	Band gaps and optical spectra from singleâ€•and doubleâ€layer fluorographene to graphite fluoride: manyâ€body effects and excitonic states. Annalen Der Physik, 2014, 526, 408-414.	2.4	49
112	Malonate-based inhibitors of mammalian serine racemase: Kinetic characterization and structure-based computational study. European Journal of Medicinal Chemistry, 2015, 89, 189-197.	5.5	49
113	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, 223-235.	2.9	48
114	Rational Design of Graphene Derivatives for Electrochemical Reduction of Nitrogen to Ammonia. ACS Nano, 2021, 15, 17275-17298.	14.6	48
115	Hierarchical porous metalâ€“organic framework materials for efficient oilâ€“water separation. Journal of Materials Chemistry A, 2022, 10, 2751-2785.	10.3	48
116	Hairpins participating in folding of human telomeric sequence quadruplexes studied by standard and T-REMD simulations. Nucleic Acids Research, 2015, 43, gkv994.	14.5	47
117	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.	5.3	47
118	2D Chemistry: Chemical Control of Graphene Derivatization. Journal of Physical Chemistry Letters, 2018, 9, 3580-3585.	4.6	47
119	Unique cellular network formation guided by heterostructures based on reduced graphene oxide - Ti3C2Tx MXene hydrogels. Acta Biomaterialia, 2020, 115, 104-115.	8.3	47
120	Different Mechanisms of CDK5 and CDK2 Activation as Revealed by CDK5/p25 and CDK2/Cyclin A Dynamics. Journal of Biological Chemistry, 2006, 281, 7271-7281.	3.4	46
121	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, 11177-11187.	2.6	46
122	Fluorographites (CF_x)_n Exhibit Improved Heterogeneous Electronâ€Transfer Rates with Increasing Level of Fluorination: Towards the Sensing of Biomolecules. Chemistry - A European Journal, 2014, 20, 6665-6671.	3.3	46
123	Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy. Physical Chemistry Chemical Physics, 2014, 16, 20915-20923.	2.8	46
124	Structural Changes in Ceramide Bilayers Rationalize Increased Permeation through Stratum Corneum Models with Shorter Acyl Tails. Journal of Physical Chemistry B, 2015, 119, 9811-9819.	2.6	46
125	Metal Halide Perovskite@Metalâ€Organic Framework Hybrids: Synthesis, Design, Properties, and Applications. Small, 2020, 16, e2004891.	10.0	46
126	Interaction of Graphene and Arenes with Noble Metals. Journal of Physical Chemistry C, 2012, 116, 14151-14162.	3.1	45

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127	How to understand quantum chemical computations on DNA and RNA systems? A practical guide for non-specialists. Methods, 2013, 64, 3-11.	3.8	45
128	Reactive Conformation of the Active Site in the Hairpin Ribozyme Achieved by Molecular Dynamics Simulations with Îµ/Î¶ Force Field Reparametrizations. Journal of Physical Chemistry B, 2015, 119, 4220-4229.	2.6	45
129	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, 2101-2109.	5.3	44
130	Exact roles of individual chemical forms of nitrogen in the photoluminescent properties of nitrogen-doped carbon dots. Applied Materials Today, 2017, 7, 190-200.	4.3	44
131	Molecular Mechanism of preQ₁ Riboswitch Action: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2012, 116, 12721-12734.	2.6	43
132	Organic adsorbates have higher affinities to fluorographene than to graphene. Applied Materials Today, 2016, 5, 142-149.	4.3	43
133	The Hallmarks of Copper Single Atom Catalysts in Direct Alcohol Fuel Cells and Electrochemical CO₂ Fixation. Advanced Materials Interfaces, 2021, 8, 2001822.	3.7	43
134	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, 1872-1879.	2.6	42
135	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.	14.5	42
136	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.	5.3	41
137	Structure, dynamical stability, and electronic properties of phases in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>TaS</mml:mtext><mml:mn>2</mml:mn></mml:msub> a high-level quantum mechanical calculation. Physical Review B, 2015, 92, .	3.2	40
138	Single Coâ€Atoms as Electrocatalysts for Efficient Hydrazine Oxidation Reaction. Small, 2021, 17, e2006477.	10.0	40
139	Functionally relevant motions of haloalkane dehalogenases occur in the specificity-modulating cap domains. Protein Science, 2002, 11, 1206-1217.	7.6	40
140	Random Phase Approximation in Surface Chemistry: Water Splitting on Iron. Journal of Chemical Theory and Computation, 2013, 9, 3670-3676.	5.3	39
141	The Role of Protein-Protein and Protein-Membrane Interactions on P450 Function. Drug Metabolism and Disposition, 2016, 44, 576-590.	3.3	39
142	Exploring the Dynamics of Propeller Loops in Human Telomeric DNA Quadruplexes Using Atomistic Simulations. Journal of Chemical Theory and Computation, 2017, 13, 2458-2480.	5.3	39
143	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.	5.3	39
144	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, 445-451.	7.6	38

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145	Lipid Enhanced Exfoliation for Production of Graphene Nanosheets. Journal of Physical Chemistry C, 2013, 117, 11800-11803.	3.1	38
146	The nature of high surface energy sites in graphene and graphite. Carbon, 2014, 73, 448-453.	10.3	38
147	Highâ€Performance Supercapacitors Based on a Zwitterionic Network of Covalently Functionalized Graphene with Iron Tetraaminophthalocyanine. Advanced Functional Materials, 2018, 28, 1801111.	14.9	38
148	Positive and Negative Effects of Dopants toward Electrocatalytic Activity of MoS₂ and WS₂: Experiments and Theory. ACS Applied Materials & Interfaces, 2020, 12, 20383-20392.	8.0	38
149	Tailoring Ï€-conjugation and vibrational modes to steer on-surface synthesis of pentalene-bridged ladder polymers. Nature Communications, 2020, 11, 4567.	12.8	36
150	Accurate surface energies from first principles. Physical Review B, 2015, 91, .	3.2	35
151	Carbon Dots Detect Water-to-Ice Phase Transition and Act as Alcohol Sensors via Fluorescence Turn-Off/On Mechanism. ACS Nano, 2021, 15, 6582-6593.	14.6	34
152	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, 18, 2642-2656.	5.3	34
153	QM/MM Studies of Hairpin Ribozyme Self-Cleavage Suggest the Feasibility of Multiple Competing Reaction Mechanisms. Journal of Physical Chemistry B, 2011, 115, 13911-13924.	2.6	33
154	Benchmark quantum-chemical calculations on a complete set of rotameric families of the DNA sugarâ€“phosphate backbone and their comparison with modern density functional theory. Physical Chemistry Chemical Physics, 2013, 15, 7295.	2.8	33
155	Antiallergic Effects of Pigments Isolated from Green Sea Urchin (Strongylocentrotus droebachiensis) Shells. Planta Medica, 2013, 79, 1698-1704.	1.3	33
156	Are Waters around RNA More than Just a Solvent? â€“ An Insight from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 401-411.	5.3	33
157	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, 6423-6432.	2.8	33
158	Palladium nanoparticles supported on graphene acid: a stable and eco-friendly bifunctional Câ€“C homo- and cross-coupling catalyst. Green Chemistry, 2019, 21, 5238-5247.	9.0	33
159	Carbon Nanotube Based Metalâ€“Organic Framework Hybrids From Fundamentals Toward Applications. Small, 2022, 18, e2104628.	10.0	33
160	Dichlorocarbeneâ€Functionalized Fluorographene: Synthesis and Reaction Mechanism. Small, 2015, 11, 3790-3796.	10.0	32
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