Ursula RÃ¶thlisberger

List of Publications by Year
in descending order

265 papers	23,638 citations	13087 68 h-index	8618 146 g-index
278 all docs	278 docs citations	278 times ranked	23268 citing authors

#	Article	IF	Citations
1	Dye-sensitized solar cells with 13% efficiency achieved through the molecular engineering of porphyrin sensitizers. Nature Chemistry, 2014, 6, 242-247.	6.6	3,982
2	Pseudo-halide anion engineering for Î±-FAPbI3 perovskite solar cells. Nature, 2021, 592, 381-385.	13.7	2,095
3	Entropic stabilization of mixed A-cation ABX₃ metal halide perovskites for high performance perovskite solar cells. Energy and Environmental Science, 2016, 9, 656-662.	15.6	1,077
4	Ionic polarization-induced currentâ€“voltage hysteresis in CH3NH3PbX3 perovskite solar cells. Nature Communications, 2016, 7, 10334.	5.8	602
5	A Hamiltonian electrostatic coupling scheme for hybrid Carâ€“Parrinello molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 6941-6947.	1.2	588
6	Vapor-assisted deposition of highly efficient, stable black-phase FAPbI ₃ perovskite solar cells. Science, 2020, 370, .	6.0	530
7	Optimization of Effective Atom Centered Potentials for London Dispersion Forces in Density Functional Theory. Physical Review Letters, 2004, 93, 153004.	2.9	489
8	New Paradigm in Molecular Engineering of Sensitizers for Solar Cell Applications. Journal of the American Chemical Society, 2009, 131, 5930-5934.	6.6	385
9	Mixed Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of Biological Systems in Ground and Electronically Excited States. Chemical Reviews, 2015, 115, 6217-6263.	23.0	352
10	Structural and electronic properties of sodium microclusters (n=2â€“20) at low and high temperatures: New insights fromabinitiomolecular dynamics studies. Journal of Chemical Physics, 1991, 94, 8129-8151.	1.2	330
11	Trajectory Surface Hopping within Linear Response Time-Dependent Density-Functional Theory. Physical Review Letters, 2007, 98, 023001.	2.9	324
12	Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. Science Advances, 2016, 2, e1601156.	4.7	307
13	Structure of nanoscale silicon clusters. Physical Review Letters, 1994, 72, 665-668.	2.9	288
14	The Role and Perspective of Ab Initio Molecular Dynamics in the Study of Biological Systems. Accounts of Chemical Research, 2002, 35, 455-464.	7.6	287
15	Ligand substitutions between rutheniumâ€“cymene compounds can control protein versus DNA targeting and anticancer activity. Nature Communications, 2014, 5, 3462.	5.8	257
16	Quantitative Photo Activated Localization Microscopy: Unraveling the Effects of Photoblinking. PLoS ONE, 2011, 6, e22678.	1.1	252
17	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamicsâ€”Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. Journal of Chemical Theory and Computation, 2012, 8, 3902-3910.	2.3	247
18	Binding of Organometallic Ruthenium(II) and Osmium(II) Complexes to an Oligonucleotide:Â A Combined Mass Spectrometric and Theoretical Studyâ€. Organometallics, 2005, 24, 2114-2123.	1.1	210

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19	Identification of clustering artifacts in photoactivated localization microscopy. Nature Methods, 2011, 8, 527-528.	9.0	197
20	Sodium cluster ionisation potentials revisited: Higher-resolution measurements for Nax (x<23) and their relation to bonding models. Chemical Physics Letters, 1988, 143, 251-258.	1.2	194
21	D-RESP:â€‰ Dynamically Generated Electrostatic Potential Derived Charges from Quantum Mechanics/Molecular Mechanics Simulations. Journal of Physical Chemistry B, 2002, 106, 7300-7307.	1.2	187
22	Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. Journal of Chemical Physics, 2008, 129, 124108.	1.2	182
23	Importance of van der Waals Interactions in Liquid Water. Journal of Physical Chemistry B, 2009, 113, 1127-1131.	1.2	175
24	Trajectoryâ€Based Nonadiabatic Dynamics with Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2013, 14, 1314-1340.	1.0	168
25	Acid-Induced Degradation of Phosphorescent Dopants for OLEDs and Its Application to the Synthesis of Tris-heteroleptic Iridium(III) Bis-cyclometalated Complexes. Inorganic Chemistry, 2012, 51, 215-224.	1.9	165
26	Influence of Hydrogen-Bonding Substituents on the Cytotoxicity of RAPTA Compounds. Organometallics, 2006, 25, 756-765.	1.1	154
27	Molecular Engineering of a Fluorene Donor for Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2733-2739.	3.2	154
28	Charge migration and charge transfer in molecular systems. Structural Dynamics, 2017, 4, 061508.	0.9	146
29	Crown Ether Modulation Enables over 23% Efficient Formamidinium-Based Perovskite Solar Cells. Journal of the American Chemical Society, 2020, 142, 19980-19991.	6.6	145
30	Microsolvation Effects on the Excited-State Dynamics of Protonated Tryptophan. Journal of the American Chemical Society, 2006, 128, 16938-16943.	6.6	144
31	Thirteenâ€atom clusters: Equilibrium geometries, structural transformations, and trends in Na, Mg, Al, and Si. Journal of Chemical Physics, 1992, 96, 1248-1256.	1.2	140
32	Role of protein frame and solvent for the redox properties of azurin from Pseudomonas aeruginosa. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 19641-19646.	3.3	135
33	Valence and conduction band tuning in halide perovskites for solar cell applications. Journal of Materials Chemistry A, 2016, 4, 15997-16002.	5.2	132
34	Molecular dynamics in electronically excited states using time-dependent density functional theory. Molecular Physics, 2005, 103, 963-981.	0.8	130
35	Drug resistance in HIV-1 protease: Flexibility-assisted mechanism of compensatory mutations. Protein Science, 2009, 11, 2393-2402.	3.1	124
36	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamicsâ€”Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. Journal of Chemical Theory and Computation, 2012, 8, 3902-3910.	2.3	116

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37	Nonadiabatic coupling vectors within linear response time-dependent density functional theory. Journal of Chemical Physics, 2009, 130, 124107.	1.2	114
38	Stabilization of the Perovskite Phase of Formamidinium Lead Triiodide by Methylammonium, Cs, and/or Rb Doping. Journal of Physical Chemistry Letters, 2017, 8, 1191-1196.	2.1	114
39	Variational Particle Number Approach for Rational Compound Design. Physical Review Letters, 2005, 95, 153002.	2.9	112
40	Early Steps of the Intramolecular Signal Transduction in Rhodopsin Explored by Molecular Dynamics Simulationsâ€. Biochemistry, 2002, 41, 10799-10809.	1.2	111
41	QM/MM Car-Parrinello Molecular Dynamics Study of the Solvent Effects on the Ground State and on the First Excited Singlet State of Acetone in Water. ChemPhysChem, 2003, 4, 1177-1182.	1.0	110
42	Variational optimization of effective atom centered potentials for molecular properties. Journal of Chemical Physics, 2005, 122, 014113.	1.2	110
43	Cisplatin Binding to DNA Oligomers from Hybrid Car-Parrinello/Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 2699-2707.	1.2	109
44	Influence of Halogen Atoms on a Homologous Series of Bis-Cyclometalated Iridium(III) Complexes. Inorganic Chemistry, 2012, 51, 799-811.	1.9	107
45	Reaction Mechanism of HIV-1 Protease by Hybrid Car-Parrinello/Classical MD Simulations. Journal of Physical Chemistry B, 2004, 108, 11139-11149.	1.2	106
46	Nonadiabatic coupling vectors for excited states within time-dependent density functional theory in the Tammâ€“Dancoff approximation and beyond. Journal of Chemical Physics, 2010, 133, 194104.	1.2	105
47	Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies. ChemMedChem, 2016, 11, 1199-1210.	1.6	104
48	Atomic-Level Microstructure of Efficient Formamidinium-Based Perovskite Solar Cells Stabilized by 5-Ammonium Valeric Acid Iodide Revealed by Multinuclear and Two-Dimensional Solid-State NMR. Journal of the American Chemical Society, 2019, 141, 17659-17669.	6.6	104
49	Nonadiabatic molecular dynamics with solvent effects: A LR-TDDFT QM/MM study of ruthenium (II) tris (bipyridine) in water. Chemical Physics, 2011, 391, 101-109.	0.9	101
50	Water-Assisted Reaction Mechanism of Monozinc Î²-Lactamases. Journal of the American Chemical Society, 2004, 126, 12661-12668.	6.6	99
51	A Molecular Spring for Vision. Journal of the American Chemical Society, 2004, 126, 15328-15329.	6.6	98
52	Predictive Determination of Band Gaps of Inorganic Halide Perovskites. Journal of Physical Chemistry Letters, 2017, 8, 5507-5512.	2.1	98
53	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. Journal of Chemical Physics, 1997, 106, 4658-4664.	1.2	95
54	DNA Structural Distortions Induced by Rutheniumâ€'Arene Anticancer Compounds. Journal of the American Chemical Society, 2008, 130, 10921-10928.	6.6	94

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55	The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. Journal of the American Chemical Society, 2015, 137, 11170-11178.	6.6	86
56	Polarization effects and charge transfer in the KcsA potassium channel. Biophysical Chemistry, 2006, 124, 292-301.	1.5	84
57	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454.	2.3	81
58	On nonadiabatic coupling vectors in time-dependent density functional theory. Journal of Chemical Physics, 2009, 131, 196101.	1.2	80
59	Directed Evolution of the Suicide Protein O⁶-Alkylguanine-DNA Alkyltransferase for Increased Reactivity Results in an Alkylated Protein with Exceptional Stability. Biochemistry, 2012, 51, 986-994.	1.2	80
60	Who Activates the Nucleophile in Ribozyme Catalysis? An Answer from the Splicing Mechanism of Group II Introns. Journal of the American Chemical Society, 2016, 138, 10374-10377.	6.6	79
61	Automated Parametrization of Biomolecular Force Fields from Quantum Mechanics/Molecular Mechanics (QM/MM) Simulations through Force Matching. Journal of Chemical Theory and Computation, 2007, 3, 628-639.	2.3	78
62	A universal co-solvent dilution strategy enables facile and cost-effective fabrication of perovskite photovoltaics. Nature Communications, 2022, 13, 89.	5.8	77
63	Cuâ€“Al Spinel as a Highly Active and Stable Catalyst for the Reverse Water Gas Shift Reaction. ACS Catalysis, 2019, 9, 6243-6251.	5.5	76
64	Evolutionarily Conserved Functional Mechanics across Pepsin-like and Retroviral Aspartic Proteases. Journal of the American Chemical Society, 2005, 127, 3734-3742.	6.6	74
65	Studies of Glutathione Transferase P1â€1 Bound to a Platinum(IV)â€Based Anticancer Compound Reveal the Molecular Basis of Its Activation. Chemistry - A European Journal, 2011, 17, 7806-7816.	1.7	73
66	pKa Estimation of Ruthenium(II)â^'Arene PTA Complexes and their Hydrolysis Products via a DFT/Continuum Electrostatics Approach. Organometallics, 2007, 26, 3969-3975.	1.1	72
67	Multimodal hostâ€“guest complexation for efficient and stable perovskite photovoltaics. Nature Communications, 2021, 12, 3383.	5.8	72
68	Canonical Adiabatic Free Energy Sampling (CAFES):â€‰ A Novel Method for the Exploration of Free Energy Surfaces. Journal of Physical Chemistry B, 2002, 106, 203-208.	1.2	70
69	A QM/MM Investigation of Thymine Dimer Radical Anion Splitting Catalyzed by DNA Photolyase. ChemPhysChem, 2009, 10, 400-410.	1.0	70
70	Nanoscale interfacial engineering enables highly stable and efficient perovskite photovoltaics. Energy and Environmental Science, 2021, 14, 5552-5562.	15.6	69
71	Formation of Boronate Ester Polymers with Efficient Intrastrand Chargeâ€Transfer Transitions by Threeâ€Component Reactions. European Journal of Inorganic Chemistry, 2007, 2007, 5177-5181.	1.0	68
72	Electron Localization Dynamics in the Triplet Excited State of [Ru(bpy)₃]²⁺ in Aqueous Solution. Chemistry - A European Journal, 2010, 16, 5889-5894.	1.7	68

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73	The Structure of the Protonated Serine Octamer. Journal of the American Chemical Society, 2018, 140, 7554-7560.	6.6	67
74	Weakly Bonded Complexes of Aliphatic and Aromatic Carbon Compounds Described with Dispersion Corrected Density Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 1673-1679.	2.3	66
75	Solvent and Protein Effects on the Structure and Dynamics of the Rhodopsin Chromophore. ChemPhysChem, 2005, 6, 1836-1847.	1.0	65
76	Coordination Numbers of K+ and Na+ Ions Inside the Selectivity Filter ofÂtheÂKcsA Potassium Channel: Insights from First Principles MolecularÂDynamics. Biophysical Journal, 2010, 98, L47-L49.	0.2	64
77	Trajectory-based solution of the nonadiabatic quantum dynamics equations: an on-the-fly approach for molecular dynamics simulations. Physical Chemistry Chemical Physics, 2011, 13, 3231.	1.3	64
78	Computational Study of Thymine Dimer Radical Anion Splitting in the Self-Repair Process of Duplex DNA. Journal of the American Chemical Society, 2008, 130, 3443-3450.	6.6	63
79	Coldâ€Ion Spectroscopy Reveals the Intrinsic Structure of a Decapeptide. Angewandte Chemie - International Edition, 2011, 50, 5383-5386.	7.2	63
80	Nanocomposites Containing Neutral Blue Emitting Cyclometalated Iridium(III) Emitters for Oxygen Sensing. Chemistry of Materials, 2012, 24, 2330-2338.	3.2	63
81	Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions. Chimia, 2002, 56, 13-19.	0.3	62
82	Predicting Noncovalent Interactions between Aromatic Biomolecules with London-Dispersion-Corrected DFT. Journal of Physical Chemistry B, 2007, 111, 14346-14354.	1.2	62
83	Non-adiabatic dynamics using time-dependent density functional theory: Assessing the coupling strengths. Computational and Theoretical Chemistry, 2009, 914, 22-29.	1.5	61
84	Tuning the Efficacy of Ruthenium(II)-Arene (RAPTA) Antitumor Compounds with Fluorinated Arene Ligands. Organometallics, 2009, 28, 5061-5071.	1.1	61
85	Combined QM/MM and Classical Molecular Dynamics Study of [Ru(bpy)₃]²⁺ in Water. Journal of Physical Chemistry B, 2009, 113, 7737-7744.	1.2	61
86	Insights into Intrastrand Cross-Link Lesions of DNA from QM/MM Molecular Dynamics Simulations. Journal of the American Chemical Society, 2012, 134, 2111-2119.	6.6	61
87	Allosteric cross-talk in chromatin can mediate drug-drug synergy. Nature Communications, 2017, 8, 14860.	5.8	61
88	Guanineâ€Stabilized Formamidinium Lead Iodide Perovskites. Angewandte Chemie - International Edition, 2020, 59, 4691-4697.	7.2	61
89	Formamidiniumâ€Based Dionâ€Jacobson Layered Hybrid Perovskites: Structural Complexity and Optoelectronic Properties. Advanced Functional Materials, 2020, 30, 2003428.	7.8	61
90	Hydrogen Bonding Described Using Dispersion-Corrected Density Functional Theory. Journal of Physical Chemistry B, 2009, 113, 4726-4732.	1.2	60

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91	Describing weak interactions of biomolecules with dispersion-corrected density functional theory. Physical Chemistry Chemical Physics, 2008, 10, 2730.	1.3	59
92	All-atom simulations disentangle the functional dynamics underlying gene maturation in the intron lariat spliceosome. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6584-6589.	3.3	59
93	Nuclear Magnetic Resonance Chemical Shifts from Hybrid DFT QM/MM Calculations. Journal of Physical Chemistry B, 2004, 108, 2807-2815.	1.2	58
94	The torsional potential of perfluoronâ€alkanes: A density functional study. Journal of Chemical Physics, 1996, 104, 3692-3700.	1.2	56
95	Hydroxide and Proton Migration in Aquaporins. Biophysical Journal, 2005, 89, 1744-1759.	0.2	56
96	Essential role of oxygen vacancies of Cu-Al and Co-Al spinel oxides in their catalytic activity for the reverse water gas shift reaction. Applied Catalysis B: Environmental, 2020, 266, 118669.	10.8	56
97	Nanoscale Phase Segregation in Supramolecular Ï€-Templating for Hybrid Perovskite Photovoltaics from NMR Crystallography. Journal of the American Chemical Society, 2021, 143, 1529-1538.	6.6	55
98	Charge transfer relaxation in donorâ€“acceptor type conjugated materials. Journal of Materials Chemistry C, 2013, 1, 2308.	2.7	54
99	Development of Site-Specific Mg²⁺â€“RNA Force Field Parameters: A Dream or Reality? Guidelines from Combined Molecular Dynamics and Quantum Mechanics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 340-352.	2.3	51
100	Reactions of Alkynes with [RuCl(cyclopentadienyl)] Complexes: The Important First Steps. Chemistry - A European Journal, 2010, 16, 8400-8409.	1.7	50
101	Mixed quantum-classical dynamics with time-dependent external fields: A time-dependent density-functional-theory approach. Physical Review A, 2010, 81, .	1.0	49
102	Unravelling the Potential for Dithienopyrrole Sensitizers in Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2642-2648.	3.2	49
103	A combined molecular dynamics and experimental study of two-step process enabling low-temperature formation of phase-pure Î±-FAPbI ₃. Science Advances, 2021, 7, .	4.7	49
104	Synthesis, characterization and ab initio investigation of a panchromatic ullazineâ€“porphyrin photosensitizer for dye-sensitized solar cells. Journal of Materials Chemistry A, 2016, 4, 2332-2339.	5.2	47
105	Ditantalum Hydride Complexes with Bridging (2,6-iPr2C6H3)NSiHPh Silanimine Ligands Resulting from PhSiH3â"Imido Ligand Coupling. A Combined Spectroscopic and Theoretical Investigation. Organometallics, 2000, 19, 3830-3841.	1.1	45
106	Effect of graphene oxide nanosheets on visible light-assisted antibacterial activity of vertically-aligned copper oxide nanowire arrays. Journal of Colloid and Interface Science, 2018, 521, 119-131.	5.0	45
107	Atomistic Mechanism of the Nucleation of Methylammonium Lead Iodide Perovskite from Solution. Chemistry of Materials, 2020, 32, 529-536.	3.2	45
108	Characterization of the Dizinc Analogue of the Synthetic Diiron Protein DF1 Using ab Initio and Hybrid Quantum/Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2003, 107, 4182-4188.	1.2	43

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109	Origin of the Spectral Shifts among the Early Intermediates of the Rhodopsin Photocycle. Journal of the American Chemical Society, 2014, 136, 3842-3851.	6.6	42
110	Accuracy of Molecular Simulation-Based Predictions of k_{off} Values: A Metadynamics Study. Journal of Physical Chemistry Letters, 2020, 11, 6373-6381.	2.1	41
111	Na6Pb: a bimetallic cluster of striking stability. Chemical Physics Letters, 1995, 237, 334-338.	1.2	40
112	Structure of Solid Poly(tetrafluoroethylene):â€‰ A Computer Simulation Study of Chain Orientational, Translational, and Conformational Disorder. Journal of Physical Chemistry B, 1997, 101, 2745-2749.	1.2	40
113	Dialkyl Effect on Enantioselectivity:Â Ï€-Stacking as a Structural Feature in P,N Complexes of Palladium(II). Organometallics, 2002, 21, 3033-3041.	1.1	40
114	A Variational Definition of Electrostatic Potential Derived Charges. Journal of Physical Chemistry B, 2004, 108, 7963-7968.	1.2	40
115	Computational insights into function and inhibition of fatty acid amide hydrolase. European Journal of Medicinal Chemistry, 2015, 91, 15-26.	2.6	40
116	Probing the electronic and geometric structure of ferric and ferrous myoglobins in physiological solutions by Fe K-edge absorption spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 1617-1631.	1.3	39
117	Direct observation of an equilibrium between two anion-cation orientations in olefin Pt(II) complex ion pairs by HOESY NMR spectroscopyElectronic supplementary information (ESI) available: details of the experimental measurements and calculations, along with the NMR intramolecular characterization of complexes 1â€“3. See http://www.rsc.org/suppdata/nj/b2/b212088g/. New Journal of Chemistry, 2003, 27, 455-458.	1.4	38
118	Optical Spectra of Cu(II)â^'Azurin by Hybrid TDDFT-Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 10248-10252.	1.2	38
119	The Protonation State of the Glu-71/Asp-80 Residues in the KcsA Potassium Channel: A First-Principles QM/MM Molecular Dynamics Study. Biophysical Journal, 2007, 93, 2315-2324.	0.2	38
120	Accurate DFT Descriptions for Weak Interactions of Molecules Containing Sulfur. Journal of Chemical Theory and Computation, 2009, 5, 23-28.	2.3	38
121	Predicting Novel Binding Modes of Agonists to Î² Adrenergic Receptors Using All-Atom Molecular Dynamics Simulations. PLoS Computational Biology, 2011, 7, e1001053.	1.5	38
122	Computational Characterization of the Dependence of Halide Perovskite Effective Masses on Chemical Composition and Structure. Journal of Physical Chemistry C, 2017, 121, 23886-23895.	1.5	38
123	Conformational and orientational order and disorder in solid polytetrafluoroethylene. Molecular Physics, 1999, 97, 355-373.	0.8	37
124	The Role of Ï€â^'Ï€ Stacking Interactions in Square Planar Palladium Complexes. Combined Quantum Mechanics/Molecular Mechanics QM/MM Studies. Organometallics, 2001, 20, 4178-4184.	1.1	37
125	A comparative theoretical study of dipeptide solvation in water. Journal of Computational Chemistry, 2006, 27, 672-684.	1.5	37
126	A Conserved Protonation-Induced Switch can Trigger â€œIonic-Lockâ€•Formation in Adrenergic Receptors. Journal of Molecular Biology, 2010, 397, 1339-1349.	2.0	36

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127	Anandamide Hydrolysis in FAAH Reveals a Dual Strategy for Efficient Enzyme-Assisted Amide Bond Cleavage via Nitrogen Inversion. Journal of Physical Chemistry B, 2015, 119, 789-801.	1.2	36
128	Molecular simulations of ion channels: a quantum chemistâ€™s perspective. Journal of General Physiology, 2010, 135, 549-554.	0.9	35
129	A Vibronic Coupling Hamiltonian to Describe the Ultrafast Excited State Dynamics of a Cu(I)-Phenanthroline Complex. Chimia, 2014, 68, 227.	0.3	35
130	Ruddlesdenâ€“Popper Phases of Methylammonium-Based Two-Dimensional Perovskites with 5-Ammonium Valeric Acid AVA₂MA_{nâ€“1}Pb_nI_{3n+1} with n = 1, 2, and 3. Journal of Physical Chemistry Letters, 2019, 10, 3543-3549.	2.1	35
131	Ab initio molecular dynamics studies of a synthetic biomimetic model of galactose oxidase. International Journal of Quantum Chemistry, 1999, 73, 209-218.	1.0	34
132	Enantioselective Palladium-Catalyzed Hydrosilylation of Styrene:Â Detailed Reaction Mechanism from First-Principles and Hybrid QM/MM Molecular Dynamics Simulations. Organometallics, 2004, 23, 3218-3227.	1.1	34
133	Quantum Mechanical/Molecular Mechanical (QM/MM) Car-Parrinello Simulations in Excited States. Chimia, 2005, 59, 493-498.	0.3	34
134	NMR Solvent Shifts of Adenine in Aqueous Solution from Hybrid QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 5225-5232.	1.2	34
135	Parameterization of azoleâ€bridged dinuclear platinum anticancer drugs via a QM/MM force matching procedure. Journal of Computational Chemistry, 2008, 29, 38-49.	1.5	34
136	Binding of Organometallic Ruthenium(II) Anticancer Compounds to Nucleobases: A Computational Study. Journal of Physical Chemistry A, 2009, 113, 11888-11897.	1.1	34
137	Does Proton Conduction in the Voltage-Gated H⁺ Channel hHv1 Involve Grotthuss-Like Hopping via Acidic Residues?. Journal of Physical Chemistry B, 2017, 121, 3340-3351.	1.2	34
138	Chiral Palladium(II)â^'Bis(trichlorosilyl) Complexes. Synthesis, Structure, and Combined QM/MM Computational Studies. Organometallics, 2000, 19, 2144-2152.	1.1	33
139	Rational Design of Organo-Ruthenium Anticancer Compounds. Chimia, 2005, 59, 81-84.	0.3	33
140	Integrating computational methods to retrofit enzymes to synthetic pathways. Biotechnology and Bioengineering, 2012, 109, 572-582.	1.7	32
141	Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. Journal of Chemical Theory and Computation, 2019, 15, 5601-5613.	2.3	32
142	Nonadiabatic effects in electronic and nuclear dynamics. Structural Dynamics, 2017, 4, 061510.	0.9	31
143	MiMiC: A Novel Framework for Multiscale Modeling in Computational Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 3810-3823.	2.3	31
144	Keys to Lipid Selection in Fatty Acid Amide Hydrolase Catalysis: Structural Flexibility, Gating Residues and Multiple Binding Pockets. PLoS Computational Biology, 2015, 11, e1004231.	1.5	31

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145	Efficient multidimensional free energy calculations for ab initio molecular dynamics using classical bias potentials. Journal of Chemical Physics, 2000, 113, 4863.	1.2	30
146	In Situ Mapping of the Molecular Arrangement of Amphiphilic Dye Molecules at the TiO₂ Surface of Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 10834-10842.	4.0	30
147	Oxidation of Nitrite by Peroxynitrous Acid. Journal of Physical Chemistry A, 2003, 107, 1763-1769.	1.1	29
148	Green Oxidation Catalysts: Computational Design of High-Efficiency Models of Galactose Oxidase. Angewandte Chemie - International Edition, 2004, 43, 3286-3289.	7.2	29
149	Unusual Arâ^'H/Rhâ^'HJHHNMR Coupling in Complexes of Rhodium(III):Â Experimental Evidence and Theoretical Support for an Î·1â^'Arene Structure. Journal of the American Chemical Society, 2004, 126, 12492-12502.	6.6	29
150	Ab initio molecular dynamics simulations of the gas-phase reaction of hydroxyl radical with nitrogen dioxide radical. Chemical Physics Letters, 1998, 297, 205-210.	1.2	28
151	Influence of Long-Range Electrostatic Treatments on the Folding of the N-Terminal H4 Histone Tail Peptide. Journal of Chemical Theory and Computation, 2006, 2, 246-250.	2.3	28
152	In situparameterisation of SCC-DFTB repulsive potentials by iterative Boltzmann inversion. Molecular Physics, 2013, 111, 3595-3607.	0.8	28
153	Methylammonium Triiodide for Defect Engineering of High-Efficiency Perovskite Solar Cells. ACS Energy Letters, 2021, 6, 3650-3660.	8.8	28
154	Metal clusters with impurities: NanMg (n=6â^'9, 18). Chemical Physics Letters, 1992, 198, 478-482.	1.2	27
155	Role of Environment for Catalysis of the DNA Repair Enzyme MutY. Journal of the American Chemical Society, 2012, 134, 8608-8616.	6.6	27
156	Duocarmycins Binding to DNA Investigated by Molecular Simulationâ€. Journal of Physical Chemistry B, 2006, 110, 3647-3660.	1.2	26
157	On the proton transfer mechanism in ammonia-bridged 7-hydroxyquinoline: a TDDFT molecular dynamics study. Physical Chemistry Chemical Physics, 2009, 11, 4549.	1.3	26
158	Enantioselective Palladium-Catalyzed Hydrosilylation of Styrene:Â Influence of Electronic and Steric Effects on Enantioselectivity and Catalyst Design via Hybrid QM/MM Molecular Dynamics Simulations. Organometallics, 2006, 25, 1151-1157.	1.1	25
159	Structural and Energetic Properties of Organometallic Ruthenium(II) Diamine Anticancer Compounds and Their Interaction with Nucleobases. Journal of Chemical Theory and Computation, 2007, 3, 1212-1222.	2.3	25
160	Simulations of X-ray absorption spectra: the effect of the solvent. Physical Chemistry Chemical Physics, 2012, 14, 9444.	1.3	25
161	Wagging the Tail: Essential Role of Substrate Flexibility in FAAH Catalysis. Journal of Chemical Theory and Computation, 2013, 9, 1202-1213.	2.3	24
162	Intricacies of Describing Weak Interactions Involving Halogen Atoms within Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 955-964.	2.3	24

#	ARTICLE	IF	CITATIONS
163	Implications of short time scale dynamics on long time processes. Structural Dynamics, 2017, 4, 061507.	0.9	24
164	A Versatile Multiple Time Step Scheme for Efficient ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 2834-2842.	2.3	24
165	Atomistic Origins of the Limited Phase Stability of Cs⁺-Rich FA_xCs_(1â€“x)Pbl₃ Mixtures. Chemistry of Materials, 2020, 32, 2605-2614.	3.2	24
166	Conformational Equilibria of Peroxynitrous Acid in Water:Â A First-Principles Molecular Dynamics Study. Journal of Physical Chemistry A, 2000, 104, 6464-6469.	1.1	23
167	Ultrafast Relaxation Dynamics of the Ethylene Cation C₂H₄⁺. Journal of Physical Chemistry Letters, 2016, 7, 1901-1906.	2.1	23
168	The performance of density functional methods for the description of weak interaction potentials. The torsional potential of butane. Chemical Physics Letters, 1994, 227, 390-395.	1.2	22
169	Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems. Chimia, 2011, 65, 667.	0.3	22
170	Recent Advances in First-Principles Based Molecular Dynamics. Accounts of Chemical Research, 2022, 55, 221-230.	7.6	22
171	First-Principles Simulations of Câ^'S Bond Cleavage in Rhenium Thioether Complexes. Journal of Physical Chemistry A, 2004, 108, 2008-2013.	1.1	21
172	Copper binding sites in the Câ€terminal domain of mouse prion protein: A hybrid (QM/MM) molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1084-1098.	1.5	21
173	Ab Initio Excited State Properties and Dynamics of a Prototype Ïƒ-Bridged-Donorâ^'Acceptor Molecule. Journal of Physical Chemistry A, 2009, 113, 9595-9602.	1.1	21
174	Generalized QM/MM Force Matching Approach Applied to the 11-cis Protonated Schiff Base Chromophore of Rhodopsin. Journal of Chemical Theory and Computation, 2014, 10, 412-422.	2.3	21
175	An Organometallic Compound which Exhibits a DNA Topologyâ€Dependent Oneâ€Stranded Intercalation Mode. Angewandte Chemie - International Edition, 2016, 55, 7441-7444.	7.2	21
176	Living polymers Ab initio molecular dynamics study of the initiation step in the polymerization of isoprene induced by ethyl lithium. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 501-508.	1.7	20
177	Electronically and Sterically Induced Structural Distortions in Square-Planar d8 Complexes. Organometallics, 2000, 19, 3591-3596.	1.1	20
178	Accelerating Rare Reactive Events by Means of a Finite Electronic Temperature. Journal of the American Chemical Society, 2002, 124, 8163-8171.	6.6	20
179	A Simple Approach to Room Temperature Phosphorescent Allenylidene Complexes. Angewandte Chemie - International Edition, 2012, 51, 8030-8033.	7.2	20
180	Molecular Basis of CLC Antiporter Inhibition by Fluoride. Journal of the American Chemical Society, 2020, 142, 7254-7258.	6.6	20

#	Article	IF	Citations
181	Bismuthene as a versatile photocatalyst operating under variable conditions for the photoredox C H bond functionalization. Applied Catalysis B: Environmental, 2022, 304, 120957.	10.8	20
182	CNDOL: A fast and reliable method for the calculation of electronic properties of very large systems. Applications to retinal binding pocket in rhodopsin and gas phase porphine. Journal of Chemical Physics, 2007, 127, 145102.	1.2	19
183	Study of the Redox Properties of Singlet and Triplet Tris(2,2â€²-bipyridine)ruthenium(II) ([Ru(bpy)₃]²⁺) in Aqueous Solution by Full Quantum and Mixed Quantum/Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2014, 118, 3950-3959.	1.2	19
184	Vertical Ionization Energies and Electron Affinities of Native and Damaged DNA Bases, Nucleotides, and Pairs from Density Functional Theory Calculations: Model Assessment and Implications for DNA Damage Recognition and Repair. Journal of Chemical Theory and Computation, 2019, 15, 2042-2052.	2.3	19
185	Reversible Pressureâ€Dependent Mechanochromism of Dionâ€“Jacobson and Ruddlesdenâ€“Popper Layered Hybrid Perovskites. Advanced Materials, 2022, 34, e2108720.	11.1	19
186	Theoretical Studies of the Reductive Câ€“S Bond Cleavage in Complexes of the Form [M(9S3)2]2+ (M = Re,) Tj ETQq0 0 0 rgBT /Overlock	1.1	18
187	Two Misfolding Routes for the Prion Protein around pH 4.5. PLoS Computational Biology, 2013, 9, e1003057.	1.5	18
188	Effect of N-Terminal Myristoylation on the Active Conformation of Gα_{i1}â€“GTP. Biochemistry, 2017, 56, 271-280.	1.2	18
189	Protonation of the Chromophore in the Photoactive Yellow Protein. Journal of Physical Chemistry B, 2007, 111, 3765-3773.	1.2	17
190	Developing Improved Charge Sets for the Modeling of the KcsA K⁺ Channel Using QM/MM Electrostatic Potentials. Journal of Chemical Theory and Computation, 2009, 5, 2173-2179.	2.3	17
191	Assigning the EPR Fine Structure Parameters of the Mn(II) Centers in Bacillus subtilis Oxalate Decarboxylase by Site-Directed Mutagenesis and DFT/MM Calculations. Journal of the American Chemical Society, 2014, 136, 2313-2323.	6.6	17
192	Exploring the inhibition mechanism of adenylyl cyclase type 5 by n-terminal myristoylated Gα_{i1}. PLoS Computational Biology, 2017, 13, e1005673.	1.5	17
193	Structure-Based Thermodynamic Analysis of Caspases Reveals Key Residues for Dimerization and Activityâ€. Biochemistry, 2003, 42, 8720-8728.	1.2	16
194	Genetic Algorithm Based Design and Experimental Characterization of a Highly Thermostable Metalloprotein. Journal of the American Chemical Society, 2018, 140, 4517-4521.	6.6	16
195	Regulation of adenylyl cyclase 5 in striatal neurons confers the ability to detect coincident neuromodulatory signals. PLoS Computational Biology, 2019, 15, e1007382.	1.5	16
196	Naphthalenediimide/Formamidinium-Based Low-Dimensional Perovskites. Chemistry of Materials, 2021, 33, 6412-6420.	3.2	16
197	Multiple Steering Molecular Dynamics Applied to Water Exchange at Alkali Ions. Journal of Physical Chemistry B, 2002, 106, 13027-13032.	1.2	15
198	Dispersion Corrected Atom-Centered Potentials for Phosphorus. Journal of Chemical Theory and Computation, 2009, 5, 2930-2934.	2.3	15

#	Article	IF	Citations
199	Photophysics and Photochemistry of a DNAâ€“Protein Cross-Linking Model: A Synergistic Approach Combining Experiments and Theory. Journal of Physical Chemistry B, 2014, 118, 4983-4992.	1.2	15
200	Redox Properties of Native and Damaged DNA from Mixed Quantum Mechanical/Molecular Mechanics Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 6690-6701.	2.3	15
201	Emergence of hidden phases of methylammonium lead iodide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>CH</mml:mi> upon compression. Physical Review Materials, 2018, 2, .	2.9	15
202	Hybrid Car-Parrinello/Molecular Mechanics Modelling of Transition Metal Complexes: Structure, Dynamics and Reactivity. QSAR and Combinatorial Science, 2002, 21, 119-127.	1.4	14
203	Secondary Structure Assignment of Amyloid-Î² Peptide Using Chemical Shifts. Journal of Chemical Theory and Computation, 2011, 7, 1552-1563.	2.3	14
204	Assessing the performance of computational methods for the prediction of the ground state structure of a cyclic decapeptide. International Journal of Quantum Chemistry, 2013, 113, 808-814.	1.0	14
205	Unravelling the structural complexity and photophysical properties of adamantyl-based layered hybrid perovskites. Journal of Materials Chemistry A, 2020, 8, 17732-17740.	5.2	14
206	Protonation States of Methionine Aminopeptidase and Their Relevance for Inhibitor Binding and Catalytic Activity. Journal of Biological Chemistry, 2003, 278, 47862-47867.	1.6	13
207	Low Inhibiting Power of NÂ·Â·Â·CO Based Peptidomimetic Compounds against HIV-1 Protease: Insights from a QM/MM Study. Journal of Chemical Theory and Computation, 2010, 6, 1369-1379.	2.3	13
208	Charge separation and carrier dynamics in donor-acceptor heterojunction photovoltaic systems. Structural Dynamics, 2017, 4, 061503.	0.9	13
209	Expanding the boundaries of ligandâ€“target modeling by exascale calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1535.	6.2	13
210	Three- and Four-Center Trans Effects in Triply Bonded Ditungsten Complexes:Â An ab Initio Molecular Dynamics Study of Compounds with Stoichiometry W2Cl4(NHEt)2(PMe3)2. Inorganic Chemistry, 2000, 39, 5553-5560.	1.9	12
211	Molecular Origin of the Asymmetric Photoluminescence Spectra of CsPbBr₃ at Low Temperature. Journal of Physical Chemistry Letters, 2021, 12, 2699-2704.	2.1	12
212	Kinetics and energeticsÂof metal halide perovskite conversion reactions at the nanoscale. Communications Materials, 2022, 3, .	2.9	12
213	Ultrafast anisotropic x-ray scattering in the condensed phase. New Journal of Physics, 2012, 14, 113002.	1.2	11
214	Extended Intermolecular Interactions Governing Photocurrentâ€“Voltage Relations in Ternary Organic Solar Cells. Journal of Physical Chemistry Letters, 2016, 7, 3936-3944.	2.1	11
215	Association of Both Inhibitory and Stimulatory GÎ± Subunits Implies Adenylyl Cyclase 5 Deactivation. Biochemistry, 2019, 58, 4317-4324.	1.2	11
216	15 Years of Car-Parrinello Simulations in Physics, Chemistry and Biology. Computational Chemistry - Reviews of Current Trends, 2001, , 33-68.	0.4	10

#	Article	IF	Citations
217	How Rhodopsin Tunes the Equilibrium between Protonated and Deprotonated Forms of the Retinal Chromophore. Journal of Chemical Theory and Computation, 2017, 13, 4524-4534.	2.3	10
218	Local Control Theory in Trajectory Surface Hopping Dynamics Applied to the Excitedâ€State Proton Transfer of 4â€Hydroxyacridine. ChemPhysChem, 2015, 16, 2127-2133.	1.0	9
219	Plane-Wave Implementation and Performance of Ã-la-Carte Coulomb-Attenuated Exchange-Correlation Functionals for Predicting Optical Excitation Energies in Some Notorious Cases. Journal of Chemical Theory and Computation, 2018, 14, 3184-3195.	2.3	9
220	Competing interactions in self-assembled monolayers containing peptide groups: molecular dynamics studies of long-chain perfluoro mercaptans on Au(111). Journal of Materials Chemistry, 1994, 4, 793-803.	6.7	8
221	Cisâ^'TransIsomerization in Triply-Bonded Ditungsten Complexes:Â A Multitude of Possible Pathways. Inorganic Chemistry, 2001, 40, 5780-5786.	1.9	8
222	Scanning Reactive Pathways with Orbital Biased Molecular Dynamics. Journal of Chemical Theory and Computation, 2005, 1, 554-560.	2.3	8
223	Exploiting Coordinate Scaling Relations To Accelerate Exact Exchange Calculations. Journal of Physical Chemistry Letters, 2018, 9, 3886-3890.	2.1	8
224	Atom-Centered Potentials to Describe Dispersion Forces in Density Functional Theory. Chimia, 2008, 62, 231.	0.3	7
225	Photodynamics of Lys+-Trp protein motifs: Hydrogen bonds ensure photostability. Faraday Discussions, 2013, 163, 189.	1.6	7
226	Mechanism to Trigger Unfolding in O⁶â€Alkylguanineâ€DNA Alkyltransferase. ChemBioChem, 2013, 14, 703-710.	1.3	7
227	Ab Initio and Hybrid Molecular Dynamics Simulations of the Active Site of Human Carbonic Anhydrase II: A Test Case Study. ACS Symposium Series, 1998, , 264-274.	0.5	6
228	Molecular dynamics simulations of structural changes during procaspase 3 activation. Proteins: Structure, Function and Bioinformatics, 2004, 55, 932-941.	1.5	6
229	Nonadiabatic ab initio molecular dynamics using linear-response time-dependent density functional theory. Open Physics, 2013, 11, .	0.8	6
230	Local Control Theory using Trajectory Surface Hopping and Linear-Response Time-Dependent Density Functional Theory. Chimia, 2013, 67, 218-221.	0.3	6
231	Shedding Light on the Basis Set Dependence of the Minnesota Functionals: Differences Between Plane Waves, Slater Functions, and Gaussians. Journal of Chemical Theory and Computation, 2019, 15, 557-571.	2.3	6
232	Organic Spacers in 2D Perovskites: General Trends and Structureâ€Property Relationships from Computational Studies. Helvetica Chimica Acta, 2021, 104, e2000232.	1.0	6
233	Mechanical (QM/MM) Simulations of Adiabatic and Nonadiabatic Ultrafast Phenomena. Chimia, 2011, 65, 330-333.	0.3	5
234	Excited State Dynamics with Quantum Trajectories. Chimia, 2012, 66, 174.	0.3	5

#	ARTICLE	IF	CITATIONS
235	From a week to less than a day: Speedup and scaling of coordinate-scaled exact exchange calculations in plane waves. Computer Physics Communications, 2020, 247, 106943.	3.0	5
236	MiMiC: Multiscale Modeling in Computational Chemistry. Frontiers in Molecular Biosciences, 2020, 7, 45.	1.6	5
237	GÎ±i1 inhibition mechanism of ATP-bound adenylyl cyclase type 5. PLoS ONE, 2021, 16, e0245197.	1.1	5
238	Folding pathways for initiator and effector procaspases from computer simulations. Proteins: Structure, Function and Bioinformatics, 2005, 59, 765-772.	1.5	4
239	Lessons from Nature: Computational Design of Biomimetic Compounds and Processes. Chimia, 2014, 68, 642.	0.3	4
240	Cryogenic Spectroscopy and Quantum Molecular Dynamics Determine the Structure of Cyclic Intermediates Involved in Peptide Sequence Scrambling. Journal of Physical Chemistry Letters, 2015, 6, 2524-2529.	2.1	4
241	Structural and Photophysical Templating of Conjugated Polyelectrolytes with Single-Stranded DNA. Chemistry of Materials, 2020, 32, 7347-7362.	3.2	4
242	Geneticâ€Algorithmâ€Based Optimization of a Peptidic Scaffold for Sequestration and Hydration of CO₂. ChemPhysChem, 2016, 17, 3831-3835.	1.0	3
243	Ultrafast dynamics induced by the interaction of molecules with electromagnetic fields: Several quantum, semiclassical, and classical approaches. Structural Dynamics, 2017, 4, 061509.	0.9	3
244	Ultrafast nuclear dynamics of the acetylene cation C2H2+ and its impact on the infrared probe pulse induced Câ€“H bond breaking efficiency. Physical Chemistry Chemical Physics, 2019, 21, 18380-18385.	1.3	3
245	Multidisciplinary Preclinical Investigations on Three Oxamniquine Analogues as New Drug Candidates for Schistosomiasis**. Chemistry - A European Journal, 2020, 26, 15232-15241.	1.7	3
246	A theoretical perspective of the ultrafast transient absorption dynamics of <scp>CsPbBr₃</scp>. Journal of Computational Chemistry, 2022, 43, 577-582.	1.5	3
247	Isolation of a Highly Persistent Diphosphanyl Radical: The Phosphorus Analogue of a Hydrazyl This work was supported by the ETH ZÃ¼rich and Swiss National Science Foundation.. Angewandte Chemie - International Edition, 2001, 40, 723-726.	7.2	3
248	Atom-by-Atom Synthesis of Multiatom-Supported Catalytic Clusters by Liquid-Phase Atomic Layer Deposition. ACS Sustainable Chemistry and Engineering, 2022, 10, 3455-3465.	3.2	3
249	Estimating equilibrium properties from non-Hamiltonian dynamics. Journal of Chemical Physics, 2001, 115, 7859-7864.	1.2	2
250	Advances in Density-functional-based Modeling Techniques - Recent Extensions of the Car-Parrinello Approach. Methods and Principles in Medicinal Chemistry, 2005, , 3-39.	0.3	2
251	Why choosing the right partner is important: stabilization of ternary CsyGUAxFA(1â^'yâ^'x)PbI3 perovskites. Physical Chemistry Chemical Physics, 2020, 22, 20880-20890.	1.3	2
252	Efficient Treatment of Correlation Energies at the Basis-Set Limit by Monte Carlo Summation of Continuum States. Journal of Chemical Theory and Computation, 2020, 16, 6550-6559.	2.3	2

#	Article	IF	Citations
253	Ultrafast pulse shaping modulates perceived visual brightness in living animals. Science Advances, 2021, 7, .	4.7	2
254	Biomolecular Simulation: A Perspective from High Performance Computing. Israel Journal of Chemistry, 2020, 60, 694-704.	1.0	2
255	A multiple time step algorithm for trajectory surface hopping simulations. Journal of Chemical Physics, 2022, 156, 034107.	1.2	2
256	Wavefunction-Based Electrostatic-Embedding QM/MM Using CFOUR through MiMiC. Journal of Chemical Theory and Computation, 2022, 18, 13-24.	2.3	2
257	Multiscale molecular simulations to investigate adenylyl cyclaseâ€based signaling in the brain. Wiley Interdisciplinary Reviews: Computational Molecular Science, 0, , .	6.2	2
258	QM/MM Simulation of the First Step of Vision. , 2005, , 237-243.		0
259	An Organometallic Compound which Exhibits a DNA Topologyâ€Dependent Oneâ€Stranded Intercalation Mode. Angewandte Chemie, 2016, 128, 7567-7570.	1.6	0
260	Molecular Mechanism of Chromatin Targeting by a Potent Anticancer Agent Acting at the Nucleosome Core Particle. Biophysical Journal, 2016, 110, 68a-69a.	0.2	0
261	Can Biomimetic Zinc Compounds Assist a (3 + 2) Cycloaddition Reaction? A Theoretical Perspective. Journal of Chemical Theory and Computation, 2017, 13, 6382-6390.	2.3	0
262	Guanineâ€Stabilized Formamidinium Lead Iodide Perovskites. Angewandte Chemie, 2020, 132, 4721-4727.	1.6	0
263	Molecular Dynamics Simulations of Nucleation of Lead Halide Perovskites. , 0, , .		0
264	Molecular Dynamics Simulations of Nucleation of Lead Halide Perovskites. , 0, , .		0
265	Reversible photo de-mixing in two-dimensional Dion-Jacobson mixed halide perovskites: photo-miscibility gap mapped. , 0, , .		0