Ursula RÃ¶thlisberger

List of Publications by Year
in descending order

265 papers	23,638 citations	13099 68 h-index	8396 147 g-index
278 all docs	278 docs citations	278 times ranked	23268 citing authors

#	Article	IF	Citations
1	Bismuthene as a versatile photocatalyst operating under variable conditions for the photoredox C H bond functionalization. Applied Catalysis B: Environmental, 2022, 304, 120957.	20.2	20
2	Recent Advances in First-Principles Based Molecular Dynamics. Accounts of Chemical Research, 2022, 55, 221-230.	15.6	22
3	A universal co-solvent dilution strategy enables facile and cost-effective fabrication of perovskite photovoltaics. Nature Communications, 2022, 13, 89.	12.8	77
4	A multiple time step algorithm for trajectory surface hopping simulations. Journal of Chemical Physics, 2022, 156, 034107.	3.0	2
5	A theoretical perspective of the ultrafast transient absorption dynamics of <scp>CsPbBr₃</scp>. Journal of Computational Chemistry, 2022, 43, 577-582.	3.3	3
6	Reversible Pressureâ€Dependent Mechanochromism of Dionâ€“Jacobson and Ruddlesdenâ€“Popper Layered Hybrid Perovskites. Advanced Materials, 2022, 34, e2108720.	21.0	19
7	Atom-by-Atom Synthesis of Multiatom-Supported Catalytic Clusters by Liquid-Phase Atomic Layer Deposition. ACS Sustainable Chemistry and Engineering, 2022, 10, 3455-3465.	6.7	3
8	Wavefunction-Based Electrostatic-Embedding QM/MM Using CFOUR through MiMiC. Journal of Chemical Theory and Computation, 2022, 18, 13-24.	5.3	2
9	Kinetics and energeticsÂof metal halide perovskite conversion reactions at the nanoscale. Communications Materials, 2022, 3, .	6.9	12
10	GÎ±i1 inhibition mechanism of ATP-bound adenylyl cyclase type 5. PLoS ONE, 2021, 16, e0245197.	2.5	5
11	Molecular Origin of the Asymmetric Photoluminescence Spectra of CsPbBr₃ at Low Temperature. Journal of Physical Chemistry Letters, 2021, 12, 2699-2704.	4.6	12
12	Pseudo-halide anion engineering for Î±-FAPbI3 perovskite solar cells. Nature, 2021, 592, 381-385.	27.8	2,095
13	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, .	10.3	49
14	Ultrafast pulse shaping modulates perceived visual brightness in living animals. Science Advances, 2021, 7, .	10.3	2
15	Expanding the boundaries of ligandâ€“target modeling by exascale calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1535.	14.6	13
16	Organic Spacers in 2D Perovskites: General Trends and Structureâ€Property Relationships from Computational Studies. Helvetica Chimica Acta, 2021, 104, e2000232.	1.6	6
17	Multimodal hostâ€“guest complexation for efficient and stable perovskite photovoltaics. Nature Communications, 2021, 12, 3383.	12.8	72
18	Naphthalenediimide/Formamidinium-Based Low-Dimensional Perovskites. Chemistry of Materials, 2021, 33, 6412-6420.	6.7	16

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19	Methylammonium Triiodide for Defect Engineering of High-Efficiency Perovskite Solar Cells. ACS Energy Letters, 2021, 6, 3650-3660.	17.4	28
20	Nanoscale Phase Segregation in Supramolecular Ï€-Templating for Hybrid Perovskite Photovoltaics from NMR Crystallography. Journal of the American Chemical Society, 2021, 143, 1529-1538.	13.7	55
21	Nanoscale interfacial engineering enables highly stable and efficient perovskite photovoltaics. Energy and Environmental Science, 2021, 14, 5552-5562.	30.8	69
22	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.	7.5	5
23	Atomistic Mechanism of the Nucleation of Methylammonium Lead Iodide Perovskite from Solution. Chemistry of Materials, 2020, 32, 529-536.	6.7	45
24	Guanineâ€Stabilized Formamidinium Lead Iodide Perovskites. Angewandte Chemie - International Edition, 2020, 59, 4691-4697.	13.8	61
25	Guanineâ€Stabilized Formamidinium Lead Iodide Perovskites. Angewandte Chemie, 2020, 132, 4721-4727.	2.0	0
26	Accuracy of Molecular Simulation-Based Predictions of k_{off} Values: A Metadynamics Study. Journal of Physical Chemistry Letters, 2020, 11, 6373-6381.	4.6	41
27	Formamidiniumâ€Based Dionâ€Jacobson Layered Hybrid Perovskites: Structural Complexity and Optoelectronic Properties. Advanced Functional Materials, 2020, 30, 2003428.	14.9	61
28	Structural and Photophysical Templating of Conjugated Polyelectrolytes with Single-Stranded DNA. Chemistry of Materials, 2020, 32, 7347-7362.	6.7	4
29	Unravelling the structural complexity and photophysical properties of adamantyl-based layered hybrid perovskites. Journal of Materials Chemistry A, 2020, 8, 17732-17740.	10.3	14
30	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.	5.3	15
31	Multidisciplinary Preclinical Investigations on Three Oxamniquine Analogues as New Drug Candidates for Schistosomiasis**. Chemistry - A European Journal, 2020, 26, 15232-15241.	3.3	3
32	Why choosing the right partner is important: stabilization of ternary CsyGUAxFA(1â^'yâ^'x)PbI3 perovskites. Physical Chemistry Chemical Physics, 2020, 22, 20880-20890.	2.8	2
33	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.	5.3	2
34	Crown Ether Modulation Enables over 23% Efficient Formamidinium-Based Perovskite Solar Cells. Journal of the American Chemical Society, 2020, 142, 19980-19991.	13.7	145
35	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.	20.2	56
36	Atomistic Origins of the Limited Phase Stability of Cs⁺-Rich FA_xCs_(1â€“x)PbI₃ Mixtures. Chemistry of Materials, 2020, 32, 2605-2614.	6.7	24

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37	MiMiC: Multiscale Modeling in Computational Chemistry. Frontiers in Molecular Biosciences, 2020, 7, 45.	3.5	5
38	Molecular Basis of CLC Antiporter Inhibition by Fluoride. Journal of the American Chemical Society, 2020, 142, 7254-7258.	13.7	20
39	Vapor-assisted deposition of highly efficient, stable black-phase FAPbI ₃ perovskite solar cells. Science, 2020, 370, .	12.6	530
40	Biomolecular Simulation: A Perspective from High Performance Computing. Israel Journal of Chemistry, 2020, 60, 694-704.	2.3	2
41	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.	13.7	104
42	Regulation of adenylyl cyclase 5 in striatal neurons confers the ability to detect coincident neuromodulatory signals. PLoS Computational Biology, 2019, 15, e1007382.	3.2	16
43	Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. Journal of Chemical Theory and Computation, 2019, 15, 5601-5613.	5.3	32
44	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.	2.8	3
45	Association of Both Inhibitory and Stimulatory GÎ± Subunits Implies Adenylyl Cyclase 5 Deactivation. Biochemistry, 2019, 58, 4317-4324.	2.5	11
46	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.	5.3	19
47	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.	4.6	35
48	Cuâ€“Al Spinel as a Highly Active and Stable Catalyst for the Reverse Water Gas Shift Reaction. ACS Catalysis, 2019, 9, 6243-6251.	11.2	76
49	MiMiC: A Novel Framework for Multiscale Modeling in Computational Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 3810-3823.	5.3	31
50	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.	5.3	6
51	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.	9.4	45
52	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.	5.3	9
53	A Versatile Multiple Time Step Scheme for Efficient ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 2834-2842.	5.3	24
54	The Structure of the Protonated Serine Octamer. Journal of the American Chemical Society, 2018, 140, 7554-7560.	13.7	67

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55	Genetic Algorithm Based Design and Experimental Characterization of a Highly Thermostable Metalloprotein. Journal of the American Chemical Society, 2018, 140, 4517-4521.	13.7	16
56	Exploiting Coordinate Scaling Relations To Accelerate Exact Exchange Calculations. Journal of Physical Chemistry Letters, 2018, 9, 3886-3890.	4.6	8
57	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.	7.1	59
58	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><mml:n upon compression. Physical Review Materials, 2018, 2, .	2.4	15
59	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.	4.6	114
60	Allosteric cross-talk in chromatin can mediate drug-drug synergy. Nature Communications, 2017, 8, 14860.	12.8	61
61	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.	5.3	51
62	Effect of N-Terminal Myristoylation on the Active Conformation of GÎ±_{i1}â€“GTP. Biochemistry, 2017, 56, 271-280.	2.5	18
63	Predictive Determination of Band Gaps of Inorganic Halide Perovskites. Journal of Physical Chemistry Letters, 2017, 8, 5507-5512.	4.6	98
64	Can Biomimetic Zinc Compounds Assist a (3 + 2) Cycloaddition Reaction? A Theoretical Perspective. Journal of Chemical Theory and Computation, 2017, 13, 6382-6390.	5.3	0
65	Computational Characterization of the Dependence of Halide Perovskite Effective Masses on Chemical Composition and Structure. Journal of Physical Chemistry C, 2017, 121, 23886-23895.	3.1	38
66	How Rhodopsin Tunes the Equilibrium between Protonated and Deprotonated Forms of the Retinal Chromophore. Journal of Chemical Theory and Computation, 2017, 13, 4524-4534.	5.3	10
67	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.	2.6	34
68	Nonadiabatic effects in electronic and nuclear dynamics. Structural Dynamics, 2017, 4, 061510.	2.3	31
69	Charge migration and charge transfer in molecular systems. Structural Dynamics, 2017, 4, 061508.	2.3	146
70	Ultrafast dynamics induced by the interaction of molecules with electromagnetic fields: Several quantum, semiclassical, and classical approaches. Structural Dynamics, 2017, 4, 061509.	2.3	3
71	Charge separation and carrier dynamics in donor-acceptor heterojunction photovoltaic systems. Structural Dynamics, 2017, 4, 061503.	2.3	13
72	Implications of short time scale dynamics on long time processes. Structural Dynamics, 2017, 4, 061507.	2.3	24

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73	Exploring the inhibition mechanism of adenylyl cyclase type 5 by n-terminal myristoylated GÎ±i1. PLoS Computational Biology, 2017, 13, e1005673.	3.2	17
74	An Organometallic Compound which Exhibits a DNA Topologyâ€Dependent Oneâ€Stranded Intercalation Mode. Angewandte Chemie, 2016, 128, 7567-7570.	2.0	0
75	Molecular Mechanism of Chromatin Targeting by a Potent Anticancer Agent Acting at the Nucleosome Core Particle. Biophysical Journal, 2016, 110, 68a-69a.	0.5	0
76	Ultrafast Relaxation Dynamics of the Ethylene Cation C₂H₄⁺. Journal of Physical Chemistry Letters, 2016, 7, 1901-1906.	4.6	23
77	Geneticâ€Algorithmâ€Based Optimization of a Peptidic Scaffold for Sequestration and Hydration of CO₂. ChemPhysChem, 2016, 17, 3831-3835.	2.1	3
78	Extended Intermolecular Interactions Governing Photocurrentâ€“Voltage Relations in Ternary Organic Solar Cells. Journal of Physical Chemistry Letters, 2016, 7, 3936-3944.	4.6	11
79	Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies. ChemMedChem, 2016, 11, 1199-1210.	3.2	104
80	Valence and conduction band tuning in halide perovskites for solar cell applications. Journal of Materials Chemistry A, 2016, 4, 15997-16002.	10.3	132
81	Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. Science Advances, 2016, 2, e1601156.	10.3	307
82	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.	13.7	79
83	An Organometallic Compound which Exhibits a DNA Topologyâ€Dependent Oneâ€Stranded Intercalation Mode. Angewandte Chemie - International Edition, 2016, 55, 7441-7444.	13.8	21
84	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.	10.3	47
85	Ionic polarization-induced currentâ€“voltage hysteresis in CH3NH3PbX3 perovskite solar cells. Nature Communications, 2016, 7, 10334.	12.8	602
86	Entropic stabilization of mixed A-cation ABX₃ metal halide perovskites for high performance perovskite solar cells. Energy and Environmental Science, 2016, 9, 656-662.	30.8	1,077
87	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.	2.6	36
88	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.	4.6	4
89	Mixed Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of Biological Systems in Ground and Electronically Excited States. Chemical Reviews, 2015, 115, 6217-6263.	47.7	352
90	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.	8.0	30

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91	The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. Journal of the American Chemical Society, 2015, 137, 11170-11178.	13.7	86
92	Local Control Theory in Trajectory Surface Hopping Dynamics Applied to the Excitedâ€State Proton Transfer of 4â€²-Hydroxyacridine. ChemPhysChem, 2015, 16, 2127-2133.	2.1	9
93	Computational insights into function and inhibition of fatty acid amide hydrolase. European Journal of Medicinal Chemistry, 2015, 91, 15-26.	5.5	40
94	Keys to Lipid Selection in Fatty Acid Amide Hydrolase Catalysis: Structural Flexibility, Gating Residues and Multiple Binding Pockets. PLoS Computational Biology, 2015, 11, e1004231.	3.2	31
95	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.	2.6	19
96	Lessons from Nature: Computational Design of Biomimetic Compounds and Processes. Chimia, 2014, 68, 642.	0.6	4
97	Ligand substitutions between rutheniumâ€“cymene compounds can control protein versus DNA targeting and anticancer activity. Nature Communications, 2014, 5, 3462.	12.8	257
98	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.	2.8	39
99	Dye-sensitized solar cells with 13% efficiency achieved through the molecular engineering of porphyrin sensitizers. Nature Chemistry, 2014, 6, 242-247.	13.6	3,982
100	Origin of the Spectral Shifts among the Early Intermediates of the Rhodopsin Photocycle. Journal of the American Chemical Society, 2014, 136, 3842-3851.	13.7	42
101	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.	5.3	21
102	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.	2.6	15
103	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.	13.7	17
104	A Vibronic Coupling Hamiltonian to Describe the Ultrafast Excited State Dynamics of a Cu(I)-Phenanthroline Complex. Chimia, 2014, 68, 227.	0.6	35
105	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.	2.0	14
106	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454.	5.3	81
107	Nonadiabatic ab initio molecular dynamics using linear-response time-dependent density functional theory. Open Physics, 2013, 11, .	1.7	6
108	Photodynamics of Lys+-Trp protein motifs: Hydrogen bonds ensure photostability. Faraday Discussions, 2013, 163, 189.	3.2	7

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109	In situparameterisation of SCC-DFTB repulsive potentials by iterative Boltzmann inversion. Molecular Physics, 2013, 111, 3595-3607.	1.7	28
110	Wagging the Tail: Essential Role of Substrate Flexibility in FAAH Catalysis. Journal of Chemical Theory and Computation, 2013, 9, 1202-1213.	5.3	24
111	Intricacies of Describing Weak Interactions Involving Halogen Atoms within Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 955-964.	5.3	24
112	Charge transfer relaxation in donorâ€“acceptor type conjugated materials. Journal of Materials Chemistry C, 2013, 1, 2308.	5.5	54
113	Mechanism to Trigger Unfolding in O⁶â€Alkylguanineâ€DNA Alkyltransferase. ChemBioChem, 2013, 14, 703-710.	2.6	7
114	Trajectoryâ€Based Nonadiabatic Dynamics with Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2013, 14, 1314-1340.	2.1	168
115	Molecular Engineering of a Fluorene Donor for Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2733-2739.	6.7	154
116	Unravelling the Potential for Dithienopyrrole Sensitizers in Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2642-2648.	6.7	49
117	Two Misfolding Routes for the Prion Protein around pH 4.5. PLoS Computational Biology, 2013, 9, e1003057.	3.2	18
118	Local Control Theory using Trajectory Surface Hopping and Linear-Response Time-Dependent Density Functional Theory. Chimia, 2013, 67, 218-221.	0.6	6
119	Ultrafast anisotropic x-ray scattering in the condensed phase. New Journal of Physics, 2012, 14, 113002.	2.9	11
120	Excited State Dynamics with Quantum Trajectories. Chimia, 2012, 66, 174.	0.6	5
121	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.	2.5	80
122	Insights into Intrastrand Cross-Link Lesions of DNA from QM/MM Molecular Dynamics Simulations. Journal of the American Chemical Society, 2012, 134, 2111-2119.	13.7	61
123	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.	4.0	165
124	Simulations of X-ray absorption spectra: the effect of the solvent. Physical Chemistry Chemical Physics, 2012, 14, 9444.	2.8	25
125	Role of Environment for Catalysis of the DNA Repair Enzyme MutY. Journal of the American Chemical Society, 2012, 134, 8608-8616.	13.7	27
126	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.	5.3	247

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127	Nanocomposites Containing Neutral Blue Emitting Cyclometalated Iridium(III) Emitters for Oxygen Sensing. Chemistry of Materials, 2012, 24, 2330-2338.	6.7	63
128	Influence of Halogen Atoms on a Homologous Series of Bis-Cyclometalated Iridium(III) Complexes. Inorganic Chemistry, 2012, 51, 799-811.	4.0	107
129	A Simple Approach to Room Temperature Phosphorescent Allenylidene Complexes. Angewandte Chemie - International Edition, 2012, 51, 8030-8033.	13.8	20
130	Integrating computational methods to retrofit enzymes to synthetic pathways. Biotechnology and Bioengineering, 2012, 109, 572-582.	3.3	32
131	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.	5.3	116
132	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.	2.8	64
133	Identification of clustering artifacts in photoactivated localization microscopy. Nature Methods, 2011, 8, 527-528.	19.0	197
134	Secondary Structure Assignment of Amyloid-Î² Peptide Using Chemical Shifts. Journal of Chemical Theory and Computation, 2011, 7, 1552-1563.	5.3	14
135	Quantitative Photo Activated Localization Microscopy: Unraveling the Effects of Photoblinking. PLoS ONE, 2011, 6, e22678.	2.5	252
136	Mechanical (QM/MM) Simulations of Adiabatic and Nonadiabatic Ultrafast Phenomena. Chimia, 2011, 65, 330-333.	0.6	5
137	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.	1.9	101
138	Coldâ€Ion Spectroscopy Reveals the Intrinsic Structure of a Decapeptide. Angewandte Chemie - International Edition, 2011, 50, 5383-5386.	13.8	63
139	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.	3.3	73
140	Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems. Chimia, 2011, 65, 667.	0.6	22
141	Predicting Novel Binding Modes of Agonists to Î² Adrenergic Receptors Using All-Atom Molecular Dynamics Simulations. PLoS Computational Biology, 2011, 7, e1001053.	3.2	38
142	Electron Localization Dynamics in the Triplet Excited State of [Ru(bpy)₃]²⁺ in Aqueous Solution. Chemistry - A European Journal, 2010, 16, 5889-5894.	3.3	68
143	Reactions of Alkynes with [RuCl(cyclopentadienyl)] Complexes: The Important First Steps. Chemistry - A European Journal, 2010, 16, 8400-8409.	3.3	50
144	Molecular simulations of ion channels: a quantum chemistâ€™s perspective. Journal of General Physiology, 2010, 135, 549-554.	1.9	35

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145	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.	3.0	105
146	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.	5.3	13
147	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.	0.5	64
148	Mixed quantum-classical dynamics with time-dependent external fields: A time-dependent density-functional-theory approach. Physical Review A, 2010, 81, .	2.5	49
149	A Conserved Protonation-Induced Switch can Trigger â€œIonic-Lockâ€•Formation in Adrenergic Receptors. Journal of Molecular Biology, 2010, 397, 1339-1349.	4.2	36
150	On nonadiabatic coupling vectors in time-dependent density functional theory. Journal of Chemical Physics, 2009, 131, 196101.	3.0	80
151	A QM/MM Investigation of Thymine Dimer Radical Anion Splitting Catalyzed by DNA Photolyase. ChemPhysChem, 2009, 10, 400-410.	2.1	70
152	Non-adiabatic dynamics using time-dependent density functional theory: Assessing the coupling strengths. Computational and Theoretical Chemistry, 2009, 914, 22-29.	1.5	61
153	Hydrogen Bonding Described Using Dispersion-Corrected Density Functional Theory. Journal of Physical Chemistry B, 2009, 113, 4726-4732.	2.6	60
154	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.	5.3	17
155	Tuning the Efficacy of Ruthenium(II)-Arene (RAPTA) Antitumor Compounds with Fluorinated Arene Ligands. Organometallics, 2009, 28, 5061-5071.	2.3	61
156	Dispersion Corrected Atom-Centered Potentials for Phosphorus. Journal of Chemical Theory and Computation, 2009, 5, 2930-2934.	5.3	15
157	Ab Initio Excited State Properties and Dynamics of a Prototype Ïƒ-Bridged-Donorâ^'Acceptor Molecule. Journal of Physical Chemistry A, 2009, 113, 9595-9602.	2.5	21
158	New Paradigm in Molecular Engineering of Sensitizers for Solar Cell Applications. Journal of the American Chemical Society, 2009, 131, 5930-5934.	13.7	385
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