Ursula Rthlisberger

List of Publications by Citations

262 papers	18,994 citations	63 h-index	132 g-index
278 ext. papers	21,412 ext. citations	7.3 avg, IF	6.88 L-index

#	Paper	IF	Citations
262	Dye-sensitized solar cells with 13% efficiency achieved through the molecular engineering of porphyrin sensitizers. *Nature Chemistry*, **2014**, 6, 242-7	17.6	3560
261	Entropic stabilization of mixed A-cation ABX3 metal halide perovskites for high performance perovskite solar cells. *Energy and Environmental Science*, **2016**, 9, 656-662	35.4	882
260	Pseudo-halide anion engineering for □FAPbI perovskite solar cells. *Nature*, **2021**, 592, 381-385	50.4	814
259	A Hamiltonian electrostatic coupling scheme for hybrid Car□Parrinello molecular dynamics simulations. *Journal of Chemical Physics*, **2002**, 116, 6941-6947	3.9	540
258	Ionic polarization-induced current-voltage hysteresis in CH3NH3PbX3 perovskite solar cells. *Nature Communications*, **2016**, 7, 10334	17.4	500
257	Optimization of effective atom centered potentials for london dispersion forces in density functional theory. *Physical Review Letters*, **2004**, 93, 153004	7.4	463
256	New paradigm in molecular engineering of sensitizers for solar cell applications. *Journal of the American Chemical Society*, **2009**, 131, 5930-4	16.4	365
255	Structural and electronic properties of sodium microclusters (n=2□0) at low and high temperatures: New insights from ab initio molecular dynamics studies. *Journal of Chemical Physics*, **1991**, 94, 8129-8151	3.9	311
254	Trajectory surface hopping within linear response time-dependent density-functional theory. *Physical Review Letters*, **2007**, 98, 023001	7.4	303
253	Mixed Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of Biological Systems in Ground and Electronically Excited States. *Chemical Reviews*, **2015**, 115, 6217-63	68.1	277
252	Structure of nanoscale silicon clusters. *Physical Review Letters*, **1994**, 72, 665-668	7.4	262
251	Vapor-assisted deposition of highly efficient, stable black-phase FAPbI perovskite solar cells. *Science*, **2020**, 370,	33.3	257
250	The role and perspective of ab initio molecular dynamics in the study of biological systems. *Accounts of Chemical Research*, **2002**, 35, 455-64	24.3	248
249	Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. *Science Advances*, **2016**, 2, e1601156	14.3	238
248	Ligand substitutions between ruthenium-cymene compounds can control protein versus DNA targeting and anticancer activity. *Nature Communications*, **2014**, 5, 3462	17.4	227
247	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamics-Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. *Journal of Chemical Theory and Computation*, **2012**, 8, 3902-10	6.4	207
246	Quantitative photo activated localization microscopy: unraveling the effects of photoblinking. *PLoS ONE*, **2011**, 6, e22678	3.7	202

245	Binding of Organometallic Ruthenium(II) and Osmium(II) Complexes to an Oligonucleotide: A Combined Mass Spectrometric and Theoretical Study. *Organometallics*, **2005**, 24, 2114-2123	3.8	198
244	Sodium cluster ionisation potentials revisited: Higher-resolution measurements for Nax (x. *Chemical Physics Letters*, **1988**, 143, 251-258	2.5	187
243	D-RESP: Dynamically Generated Electrostatic Potential Derived Charges from Quantum Mechanics/Molecular Mechanics Simulations. *Journal of Physical Chemistry B*, **2002**, 106, 7300-7307	3.4	174
242	Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. *Journal of Chemical Physics*, **2008**, 129, 124108	3.9	165
241	Importance of van der Waals interactions in liquid water. *Journal of Physical Chemistry B*, **2009**, 113, 1127-31	3.4	164
240	Identification of clustering artifacts in photoactivated localization microscopy. *Nature Methods*, **2011**, 8, 527-8	21.6	162
239	Influence of Hydrogen-Bonding Substituents on the Cytotoxicity of RAPTA Compounds. *Organometallics*, **2006**, 25, 756-765	3.8	148
238	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, 215-24	5.1	147
237	Trajectory-based nonadiabatic dynamics with time-dependent density functional theory. *ChemPhysChem*, **2013**, 14, 1314-40	3.2	143
236	Molecular Engineering of a Fluorene Donor for Dye-Sensitized Solar Cells. *Chemistry of Materials*, **2013**, 25, 2733-2739	9.6	136
235	Thirteen-atom clusters: Equilibrium geometries, structural transformations, and trends in Na, Mg, Al, and Si. *Journal of Chemical Physics*, **1992**, 96, 1248-1256	3.9	131
234	Microsolvation effects on the excited-state dynamics of protonated tryptophan. *Journal of the American Chemical Society*, **2006**, 128, 16938-43	16.4	130
233	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, 19641-6	11.5	126
232	Molecular dynamics in electronically excited states using time-dependent density functional theory. *Molecular Physics*, **2005**, 103, 963-981	1.7	120
231	Drug resistance in HIV-1 protease: Flexibility-assisted mechanism of compensatory mutations. *Protein Science*, **2002**, 11, 2393-402	6.3	105
230	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, 1177-82	3.2	105
229	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamics: 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	6.4	105
228	Variational optimization of effective atom centered potentials for molecular properties. *Journal of Chemical Physics*, **2005**, 122, 14113	3.9	104

227	Variational particle number approach for rational compound design. *Physical Review Letters*, **2005**, 95, 153002	7.4	103
226	Nonadiabatic coupling vectors within linear response time-dependent density functional theory. *Journal of Chemical Physics*, **2009**, 130, 124107	3.9	102
225	Early steps of the intramolecular signal transduction in rhodopsin explored by molecular dynamics simulations. *Biochemistry*, **2002**, 41, 10799-809	3.2	102
224	Cisplatin Binding to DNA Oligomers from Hybrid Car-Parrinello/Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 2699-2707	3.4	101
223	Reaction Mechanism of HIV-1 Protease by Hybrid Car-Parrinello/Classical MD Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 11139-11149	3.4	100
222	Charge migration and charge transfer in molecular systems. *Structural Dynamics*, **2017**, 4, 061508	3.2	98
221	Influence of halogen atoms on a homologous series of bis-cyclometalated iridium(III) complexes. *Inorganic Chemistry*, **2012**, 51, 799-811	5.1	97
220	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	6.4	96
219	Water-assisted reaction mechanism of monozinc beta-lactamases. *Journal of the American Chemical Society*, **2004**, 126, 12661-8	16.4	92
218	Valence and conduction band tuning in halide perovskites for solar cell applications. *Journal of Materials Chemistry A*, **2016**, 4, 15997-16002	13	90
217	Nonadiabatic coupling vectors for excited states within time-dependent density functional theory in the Tamm-Dancoff approximation and beyond. *Journal of Chemical Physics*, **2010**, 133, 194104	3.9	90
216	DNA structural distortions induced by ruthenium-arene anticancer compounds. *Journal of the American Chemical Society*, **2008**, 130, 10921-8	16.4	88
215	A molecular spring for vision. *Journal of the American Chemical Society*, **2004**, 126, 15328-9	16.4	88
214	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. *Journal of Chemical Physics*, **1997**, 106, 4658-4664	3.9	87
213	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	2.3	85
212	Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies. *ChemMedChem*, **2016**, 11, 1199-210	3.7	85
211	Polarization effects and charge transfer in the KcsA potassium channel. *Biophysical Chemistry*, **2006**, 124, 292-301	3.5	78
210	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, 628-39	6.4	74

209	On nonadiabatic coupling vectors in time-dependent density functional theory. *Journal of Chemical Physics*, **2009**, 131, 196101	3.9	73
208	Crown Ether Modulation Enables over 23% Efficient Formamidinium-Based Perovskite Solar Cells. *Journal of the American Chemical Society*, **2020**, 142, 19980-19991	16.4	72
207	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. *Journal of Chemical Theory and Computation*, **2013**, 9, 2441-54	6.4	71
206	Evolutionarily conserved functional mechanics across pepsin-like and retroviral aspartic proteases. *Journal of the American Chemical Society*, **2005**, 127, 3734-42	16.4	71
205	pKa Estimation of Ruthenium(II)Arene PTA Complexes and their Hydrolysis Products via a DFT/Continuum Electrostatics Approach. *Organometallics*, **2007**, 26, 3969-3975	3.8	70
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203	A QM/MM investigation of thymine dimer radical anion splitting catalyzed by DNA photolyase. *ChemPhysChem*, **2009**, 10, 400-10	3.2	67
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200	Predictive Determination of Band Gaps of Inorganic Halide Perovskites. *Journal of Physical Chemistry Letters*, **2017**, 8, 5507-5512	6.4	63
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198	Solvent and protein effects on the structure and dynamics of the rhodopsin chromophore. *ChemPhysChem*, **2005**, 6, 1836-47	3.2	62
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194	Nanocomposites Containing Neutral Blue Emitting Cyclometalated Iridium(III) Emitters for Oxygen Sensing. *Chemistry of Materials*, **2012**, 24, 2330-2338	9.6	60
193	Electron localization dynamics in the triplet excited state of [Ru(bpy)3]2+ in aqueous solution. *Chemistry - A European Journal*, **2010**, 16, 5889-94	4.8	59
192	Computational study of thymine dimer radical anion splitting in the self-repair process of duplex DNA. *Journal of the American Chemical Society*, **2008**, 130, 3443-50	16.4	59

191	Formation of Boronate Ester Polymers with Efficient Intrastrand Charge-Transfer Transitions by Three-Component Reactions. *European Journal of Inorganic Chemistry*, **2007**, 2007, 5177-5181	2.3	59
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183	Coordination numbers of K(+) and Na(+) Ions inside the selectivity filter of the KcsA potassium channel: insights from first principles molecular dynamics. *Biophysical Journal*, **2010**, 98, L47-9	2.9	55
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168	Guanine-Stabilized Formamidinium Lead Iodide Perovskites. *Angewandte Chemie - International Edition*, **2020**, 59, 4691-4697	16.4	40
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166	A Variational Definition of Electrostatic Potential Derived Charges. *Journal of Physical Chemistry B*, **2004**, 108, 7963-7968	3.4	39
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160	Direct observation of an equilibrium between two anion-cation orientations in olefin Pt(II) complex ion pairs by HOESY NMR spectroscopy. *New Journal of Chemistry*, **2003**, 27, 455-458	3.6	37
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157	CuAl Spinel as a Highly Active and Stable Catalyst for the Reverse Water Gas Shift Reaction. *ACS Catalysis*, **2019**, 9, 6243-6251	13.1	35
156	Accurate DFT Descriptions for Weak Interactions of Molecules Containing Sulfur. *Journal of Chemical Theory and Computation*, **2009**, 5, 23-8	6.4	35

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142	The Role of π Stacking Interactions in Square Planar Palladium Complexes. Combined Quantum Mechanics/Molecular Mechanics QM/MM Studies. *Organometallics*, **2001**, 20, 4178-4184	3.8	31
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