Ursula Rthlisberger

List of Publications by Year in Descending Order

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	Recent Advances in First-Principles Based Molecular Dynamics.. *Accounts of Chemical Research*, **2022**,	24.3	3
261	A universal co-solvent dilution strategy enables facile and cost-effective fabrication of perovskite photovoltaics.. *Nature Communications*, **2022**, 13, 89	17.4	14
260	A multiple time step algorithm for trajectory surface hopping simulations.. *Journal of Chemical Physics*, **2022**, 156, 034107	3.9	2
259	A theoretical perspective of the ultrafast transient absorption dynamics of CsPbBr.. *Journal of Computational Chemistry*, **2022**,	3.5	1
258	Bismuthene as a versatile photocatalyst operating under variable conditions for the photoredox CH bond functionalization. *Applied Catalysis B: Environmental*, **2022**, 304, 120957	21.8	1
257	Reversible Pressure-Dependent Mechanochromism of Dion-Jacobson and Ruddlesden-Popper Layered Hybrid Perovskites.. *Advanced Materials*, **2022**, e2108720	24	2
256	Atom-by-Atom Synthesis of Multiatom-Supported Catalytic Clusters by Liquid-Phase Atomic Layer Deposition. *ACS Sustainable Chemistry and Engineering*, **2022**, 10, 3455-3465	8.3	0
255	Pseudo-halide anion engineering for FAPbI perovskite solar cells. *Nature*, **2021**, 592, 381-385	50.4	814
254	A combined molecular dynamics and experimental study of two-step process enabling low-temperature formation of phase-pure FAPbI. *Science Advances*, **2021**, 7,	14.3	17
253	Expanding the boundaries of ligand target modeling by exascale calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1535	7.9	2
252	Organic Spacers in 2D Perovskites: General Trends and Structure-Property Relationships from Computational Studies. *Helvetica Chimica Acta*, **2021**, 104, e2000232	2	3
251	Multimodal host-guest complexation for efficient and stable perovskite photovoltaics. *Nature Communications*, **2021**, 12, 3383	17.4	17
250	GI inhibition mechanism of ATP-bound adenylyl cyclase type 5. *PLoS ONE*, **2021**, 16, e0245197	3.7	2
249	Molecular Origin of the Asymmetric Photoluminescence Spectra of CsPbBr at Low Temperature. *Journal of Physical Chemistry Letters*, **2021**, 12, 2699-2704	6.4	7
248	Naphthalenediimide/Formamidinium-Based Low-Dimensional Perovskites. *Chemistry of Materials*, **2021**, 33, 6412-6420	9.6	2
247	Nanoscale Phase Segregation in Supramolecular Templating for Hybrid Perovskite Photovoltaics from NMR Crystallography. *Journal of the American Chemical Society*, **2021**, 143, 1529-1538	16.4	26
246	Nanoscale interfacial engineering enables highly stable and efficient perovskite photovoltaics. *Energy and Environmental Science*, **2021**, 14, 5552-5562	35.4	20

245	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
244	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	21.8	24
243	Atomistic Origins of the Limited Phase Stability of Cs+-Rich FAxCs(1⊠)PbI3 Mixtures. *Chemistry of Materials*, **2020**, 32, 2605-2614	9.6	14
242	MiMiC: Multiscale Modeling in Computational Chemistry. *Frontiers in Molecular Biosciences*, **2020**, 7, 45	5.6	3
241	Molecular Basis of CLC Antiporter Inhibition by Fluoride. *Journal of the American Chemical Society*, **2020**, 142, 7254-7258	16.4	10
240	Vapor-assisted deposition of highly efficient, stable black-phase FAPbI perovskite solar cells. *Science*, **2020**, 370,	33.3	257
239	Biomolecular Simulation: A Perspective from High Performance Computing. *Israel Journal of Chemistry*, **2020**, 60, 694-704	3.4	0
238	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	4.2	3
237	Atomistic Mechanism of the Nucleation of Methylammonium Lead Iodide Perovskite from Solution. *Chemistry of Materials*, **2020**, 32, 529-536	9.6	24
236	Guanine-Stabilized Formamidinium Lead Iodide Perovskites. *Angewandte Chemie - International Edition*, **2020**, 59, 4691-4697	16.4	40
235	Guanine-Stabilized Formamidinium Lead Iodide Perovskites. *Angewandte Chemie*, **2020**, 132, 4721-4727	3.6	
234	Accuracy of Molecular Simulation-Based Predictions of Values: A Metadynamics Study. *Journal of Physical Chemistry Letters*, **2020**, 11, 6373-6381	6.4	14
233	Formamidinium-Based Dion-Jacobson Layered Hybrid Perovskites: Structural Complexity and Optoelectronic Properties. *Advanced Functional Materials*, **2020**, 30, 2003428	15.6	34
232	Structural and Photophysical Templating of Conjugated Polyelectrolytes with Single-Stranded DNA. *Chemistry of Materials*, **2020**, 32, 7347-7362	9.6	1
231	Unravelling the structural complexity and photophysical properties of adamantyl-based layered hybrid perovskites. *Journal of Materials Chemistry A*, **2020**, 8, 17732-17740	13	7
230	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	6.4	8
229	Multidisciplinary Preclinical Investigations on Three Oxamniquine Analogues as New Drug Candidates for Schistosomiasis*. *Chemistry - A European Journal*, **2020**, 26, 15232-15241	4.8	1
228	Why choosing the right partner is important: stabilization of ternary CsGUAFAPbI perovskites. *Physical Chemistry Chemical Physics*, **2020**, 22, 20880-20890	3.6	2

227	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	6.4	1
226	Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. *Journal of Chemical Theory and Computation*, **2019**, 15, 5601-5613	6.4	20
225	Ultrafast nuclear dynamics of the acetylene cation CH and its impact on the infrared probe pulse induced C-H bond breaking efficiency. *Physical Chemistry Chemical Physics*, **2019**, 21, 18380-18385	3.6	0
224	Association of Both Inhibitory and Stimulatory G Subunits Implies Adenylyl Cyclase 5 Deactivation. *Biochemistry*, **2019**, 58, 4317-4324	3.2	6
223	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	6.4	11
222	Ruddlesden-Popper Phases of Methylammonium-Based Two-Dimensional Perovskites with 5-Ammonium Valeric Acid AVAMA Pb I with n = 1, 2, and 3. *Journal of Physical Chemistry Letters*, **2019**, 10, 3543-3549	6.4	28
221	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
220	MiMiC: A Novel Framework for Multiscale Modeling in Computational Chemistry. *Journal of Chemical Theory and Computation*, **2019**, 15, 3810-3823	6.4	18
219	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	16.4	63
218	Regulation of adenylyl cyclase 5 in striatal neurons confers the ability to detect coincident neuromodulatory signals. *PLoS Computational Biology*, **2019**, 15, e1007382	5	9
217	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	6.4	5
216	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	8.3	37
215	Plane-Wave Implementation and Performance of 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	6.4	8
214	A Versatile Multiple Time Step Scheme for Efficient ab Initio Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 2834-2842	6.4	15
213	The Structure of the Protonated Serine Octamer. *Journal of the American Chemical Society*, **2018**, 140, 7554-7560	16.4	47
212	Genetic Algorithm Based Design and Experimental Characterization of a Highly Thermostable Metalloprotein. *Journal of the American Chemical Society*, **2018**, 140, 4517-4521	16.4	10
211	Exploiting Coordinate Scaling Relations To Accelerate Exact Exchange Calculations. *Journal of Physical Chemistry Letters*, **2018**, 9, 3886-3890	6.4	4
210	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	11.5	39

209	Emergence of hidden phases of methylammonium lead iodide (CH3NH3PbI3) upon compression. *Physical Review Materials*, **2018**, 2,	3.2	7
208	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
207	Allosteric cross-talk in chromatin can mediate drug-drug synergy. *Nature Communications*, **2017**, 8, 14860	17.4	54
206	Development of Site-Specific Mg(2+)-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	6.4	38
205	Effect of N-Terminal Myristoylation on the Active Conformation of G□GTP. *Biochemistry*, **2017**, 56, 271-280	3.2	14
204	Predictive Determination of Band Gaps of Inorganic Halide Perovskites. *Journal of Physical Chemistry Letters*, **2017**, 8, 5507-5512	6.4	63
203	Can Biomimetic Zinc Compounds Assist a (3 + 2) Cycloaddition Reaction? A Theoretical Perspective. *Journal of Chemical Theory and Computation*, **2017**, 13, 6382-6390	6.4	
202	Computational Characterization of the Dependence of Halide Perovskite Effective Masses on Chemical Composition and Structure. *Journal of Physical Chemistry C*, **2017**, 121, 23886-23895	3.8	28
201	How Rhodopsin Tunes the Equilibrium between Protonated and Deprotonated Forms of the Retinal Chromophore. *Journal of Chemical Theory and Computation*, **2017**, 13, 4524-4534	6.4	8
200	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	3.4	23
199	Nonadiabatic effects in electronic and nuclear dynamics. *Structural Dynamics*, **2017**, 4, 061510	3.2	22
198	Charge migration and charge transfer in molecular systems. *Structural Dynamics*, **2017**, 4, 061508	3.2	98
197	Ultrafast dynamics induced by the interaction of molecules with electromagnetic fields: Several quantum, semiclassical, and classical approaches. *Structural Dynamics*, **2017**, 4, 061509	3.2	3
196	Charge separation and carrier dynamics in donor-acceptor heterojunction photovoltaic systems. *Structural Dynamics*, **2017**, 4, 061503	3.2	8
195	Implications of short time scale dynamics on long time processes. *Structural Dynamics*, **2017**, 4, 061507	3.2	18
194	Exploring the inhibition mechanism of adenylyl cyclase type 5 by n-terminal myristoylated G□. *PLoS Computational Biology*, **2017**, 13, e1005673	5	11
193	Valence and conduction band tuning in halide perovskites for solar cell applications. *Journal of Materials Chemistry A*, **2016**, 4, 15997-16002	13	90
192	Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. *Science Advances*, **2016**, 2, e1601156	14.3	238

191	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, 10374-7	16.4	52
190	An Organometallic Compound which Exhibits a DNA Topology-Dependent One-Stranded Intercalation Mode. *Angewandte Chemie - International Edition*, **2016**, 55, 7441-4	16.4	19
189	Synthesis, characterization and ab initio investigation of a panchromatic ullazine–porphyrin photosensitizer for dye-sensitized solar cells. *Journal of Materials Chemistry A*, **2016**, 4, 2332-2339	13	44
188	Ionic polarization-induced current-voltage hysteresis in CH3NH3PbX3 perovskite solar cells. *Nature Communications*, **2016**, 7, 10334	17.4	500
187	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
186	An Organometallic Compound which Exhibits a DNA Topology-Dependent One-Stranded Intercalation Mode. *Angewandte Chemie*, **2016**, 128, 7567-7570	3.6	
185	Ultrafast Relaxation Dynamics of the Ethylene Cation C(2)H(4)+. *Journal of Physical Chemistry Letters*, **2016**, 7, 1901-6	6.4	15
184	Genetic-Algorithm-Based Optimization of a Peptidic Scaffold for Sequestration and Hydration of CO. *ChemPhysChem*, **2016**, 17, 3831-3835	3.2	2
183	Extended Intermolecular Interactions Governing Photocurrent-Voltage Relations in Ternary Organic Solar Cells. *Journal of Physical Chemistry Letters*, **2016**, 7, 3936-3944	6.4	9
182	Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies. *ChemMedChem*, **2016**, 11, 1199-210	3.7	85
181	Cryogenic Spectroscopy and Quantum Molecular Dynamics Determine the Structure of Cyclic Intermediates Involved in Peptide Sequence Scrambling. *Journal of Physical Chemistry Letters*, **2015**, 6, 2524-9	6.4	3
180	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
179	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, 10834-42	9.5	30
178	The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. *Journal of the American Chemical Society*, **2015**, 137, 11170-8	16.4	61
177	Local Control Theory in Trajectory Surface Hopping Dynamics Applied to the Excited-State Proton Transfer of 4-Hydroxyacridine. *ChemPhysChem*, **2015**, 16, 2127-33	3.2	8
176	Computational insights into function and inhibition of fatty acid amide hydrolase. *European Journal of Medicinal Chemistry*, **2015**, 91, 15-26	6.8	30
175	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	3.4	31
174	Keys to Lipid Selection in Fatty Acid Amide Hydrolase Catalysis: Structural Flexibility, Gating Residues and Multiple Binding Pockets. *PLoS Computational Biology*, **2015**, 11, e1004231	5	28

173	Ligand substitutions between ruthenium-cymene compounds can control protein versus DNA targeting and anticancer activity. *Nature Communications*, **2014**, 5, 3462	17.4	227
172	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, 1617-31	3.6	32
171	Dye-sensitized solar cells with 13% efficiency achieved through the molecular engineering of porphyrin sensitizers. *Nature Chemistry*, **2014**, 6, 242-7	17.6	3560
170	Origin of the spectral shifts among the early intermediates of the rhodopsin photocycle. *Journal of the American Chemical Society*, **2014**, 136, 3842-51	16.4	38
169	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, 412-22	6.4	19
168	Photophysics and photochemistry of a DNA-protein cross-linking model: a synergistic approach combining experiments and theory. *Journal of Physical Chemistry B*, **2014**, 118, 4983-92	3.4	12
167	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, 2313-23	16.4	17
166	A vibronic coupling hamiltonian to describe the ultrafast excited state dynamics of a Cu(i)-phenanthroline complex. *Chimia*, **2014**, 68, 227-30	1.3	30
165	Study of the redox properties of singlet and triplet Tris(2,2′-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, 3950-9	3.4	13
164	Lessons from nature: computational design of biomimetic compounds and processes. *Chimia*, **2014**, 68, 642-7	1.3	3
163	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	2.1	12
162	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. *Journal of Chemical Theory and Computation*, **2013**, 9, 2441-54	6.4	71
161	Nonadiabatic ab initio molecular dynamics using linear-response time-dependent density functional theory. *Open Physics*, **2013**, 11,	1.3	4
160	Photodynamics of Lys+-Trp protein motifs: hydrogen bonds ensure photostability. *Faraday Discussions*, **2013**, 163, 189-203; discussion 243-75	3.6	6
159	In situ parameterisation of SCC-DFTB repulsive potentials by iterative Boltzmann inversion. *Molecular Physics*, **2013**, 111, 3595-3607	1.7	24
158	Wagging the Tail: Essential Role of Substrate Flexibility in FAAH Catalysis. *Journal of Chemical Theory and Computation*, **2013**, 9, 1202-13	6.4	19
157	Intricacies of Describing Weak Interactions Involving Halogen Atoms within Density Functional Theory. *Journal of Chemical Theory and Computation*, **2013**, 9, 955-64	6.4	21
156	Charge transfer relaxation in donor–acceptor type conjugated materials. *Journal of Materials Chemistry C*, **2013**, 1, 2308	7.1	46

155	Mechanism to trigger unfolding in O(6) -alkylguanine-DNA alkyltransferase. *ChemBioChem*, **2013**, 14, 703-10	3.8	5
154	Trajectory-based nonadiabatic dynamics with time-dependent density functional theory. *ChemPhysChem*, **2013**, 14, 1314-40	3.2	143
153	Molecular Engineering of a Fluorene Donor for Dye-Sensitized Solar Cells. *Chemistry of Materials*, **2013**, 25, 2733-2739	9.6	136
152	Unravelling the Potential for Dithienopyrrole Sensitizers in Dye-Sensitized Solar Cells. *Chemistry of Materials*, **2013**, 25, 2642-2648	9.6	47
151	Two misfolding routes for the prion protein around pH 4.5. *PLoS Computational Biology*, **2013**, 9, e1003057	5	18
150	Local control theory using trajectory surface hopping and linear-response time-dependent density functional theory. *Chimia*, **2013**, 67, 218-21	1.3	6
149	Towards Compatibility between Ruthenium Sensitizers and Cobalt Electrolytes in Dye-Sensitized Solar Cells. *Angewandte Chemie*, **2013**, 125, 8893-8897	3.6	8
148	Integrating computational methods to retrofit enzymes to synthetic pathways. *Biotechnology and Bioengineering*, **2012**, 109, 572-82	4.9	30
147	Directed evolution of the suicide protein O□alkylguanine-DNA alkyltransferase for increased reactivity results in an alkylated protein with exceptional stability. *Biochemistry*, **2012**, 51, 986-94	3.2	55
146	Insights into intrastrand cross-link lesions of DNA from QM/MM molecular dynamics simulations. *Journal of the American Chemical Society*, **2012**, 134, 2111-9	16.4	57
145	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
144	Simulations of X-ray absorption spectra: the effect of the solvent. *Physical Chemistry Chemical Physics*, **2012**, 14, 9444-50	3.6	20
143	Role of environment for catalysis of the DNA repair enzyme MutY. *Journal of the American Chemical Society*, **2012**, 134, 8608-16	16.4	23
142	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
141	Nanocomposites Containing Neutral Blue Emitting Cyclometalated Iridium(III) Emitters for Oxygen Sensing. *Chemistry of Materials*, **2012**, 24, 2330-2338	9.6	60
140	Influence of halogen atoms on a homologous series of bis-cyclometalated iridium(III) complexes. *Inorganic Chemistry*, **2012**, 51, 799-811	5.1	97
139	A Simple Approach to Room Temperature Phosphorescent Allenylidene Complexes. *Angewandte Chemie*, **2012**, 124, 8154-8157	3.6	3
138	A simple approach to room temperature phosphorescent allenylidene complexes. *Angewandte Chemie - International Edition*, **2012**, 51, 8030-3	16.4	18

137	Ultrafast anisotropic x-ray scattering in the condensed phase. *New Journal of Physics*, **2012**, 14, 113002	2.9	10
136	Excited state dynamics with quantum trajectories. *Chimia*, **2012**, 66, 174-7	1.3	4
135	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
134	Identification of clustering artifacts in photoactivated localization microscopy. *Nature Methods*, **2011**, 8, 527-8	21.6	162
133	Secondary Structure Assignment of Amyloid-╫Peptide Using Chemical Shifts. *Journal of Chemical Theory and Computation*, **2011**, 7, 1552-63	6.4	13
132	Quantitative photo activated localization microscopy: unraveling the effects of photoblinking. *PLoS ONE*, **2011**, 6, e22678	3.7	202
131	Mixed quantum mechanical/molecular mechanical (QM/MM) simulations of adiabatic and nonadiabatic ultrafast phenomena. *Chimia*, **2011**, 65, 330-3	1.3	5
130	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
129	Cold-ion spectroscopy reveals the intrinsic structure of a decapeptide. *Angewandte Chemie - International Edition*, **2011**, 50, 5383-6	16.4	58
128	Studies of glutathione transferase P1-1 bound to a platinum(IV)-based anticancer compound reveal the molecular basis of its activation. *Chemistry - A European Journal*, **2011**, 17, 7806-16	4.8	66
127	Trajectory-based solution of the nonadiabatic quantum dynamics equations: an on-the-fly approach for molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2011**, 13, 3231-6	3.6	61
126	Pushing the frontiers of first-principles based computer simulations of chemical and biological systems. *Chimia*, **2011**, 65, 667-71	1.3	16
125	Predicting novel binding modes of agonists to ╠adrenergic receptors using all-atom molecular dynamics simulations. *PLoS Computational Biology*, **2011**, 7, e1001053	5	33
124	Hybrid QM/MM Simulations of Enzyme-Catalyzed DNA Repair Reactions **2010**, 517-535		2
123	Molecular simulations of ion channels: a quantum chemist℅perspective. *Journal of General Physiology*, **2010**, 135, 549-54	3.4	32
122	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
121	Low Inhibiting Power of N□□CO Based Peptidomimetic Compounds against HIV-1 Protease: Insights from a QM/MM Study. *Journal of Chemical Theory and Computation*, **2010**, 6, 1369-1379	6.4	8
120	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

119	Mixed quantum-classical dynamics with time-dependent external fields: A time-dependent density-functional-theory approach. *Physical Review A*, **2010**, 81,	2.6	45
118	A conserved protonation-induced switch can trigger "ionic-lock" formation in adrenergic receptors. *Journal of Molecular Biology*, **2010**, 397, 1339-49	6.5	30
117	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
116	Reactions of alkynes with [RuCl(cyclopentadienyl)] complexes: the important first steps. *Chemistry - A European Journal*, **2010**, 16, 8400-9	4.8	46
115	On nonadiabatic coupling vectors in time-dependent density functional theory. *Journal of Chemical Physics*, **2009**, 131, 196101	3.9	73
114	A QM/MM investigation of thymine dimer radical anion splitting catalyzed by DNA photolyase. *ChemPhysChem*, **2009**, 10, 400-10	3.2	67
113	Non-adiabatic dynamics using time-dependent density functional theory: Assessing the coupling strengths. *Computational and Theoretical Chemistry*, **2009**, 914, 22-29		56
112	Hydrogen bonding described using dispersion-corrected density functional theory. *Journal of Physical Chemistry B*, **2009**, 113, 4726-32	3.4	55
111	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, 2173-9	6.4	17
110	Tuning the Efficacy of Ruthenium(II)-Arene (RAPTA) Antitumor Compounds with Fluorinated Arene Ligands. *Organometallics*, **2009**, 28, 5061-5071	3.8	56
109	Dispersion Corrected Atom-Centered Potentials for Phosphorus. *Journal of Chemical Theory and Computation*, **2009**, 5, 2930-4	6.4	15
108	Ab initio excited state properties and dynamics of a prototype sigma-bridged-donor-acceptor molecule. *Journal of Physical Chemistry A*, **2009**, 113, 9595-602	2.8	19
107	New paradigm in molecular engineering of sensitizers for solar cell applications. *Journal of the American Chemical Society*, **2009**, 131, 5930-4	16.4	365
106	Importance of van der Waals interactions in liquid water. *Journal of Physical Chemistry B*, **2009**, 113, 1127-31	3.4	164
105	Binding of organometallic ruthenium(II) anticancer compounds to nucleobases: a computational study. *Journal of Physical Chemistry A*, **2009**, 113, 11888-97	2.8	32
104	On the proton transfer mechanism in ammonia-bridged 7-hydroxyquinoline: a TDDFT molecular dynamics study. *Physical Chemistry Chemical Physics*, **2009**, 11, 4549-55	3.6	26
103	Nonadiabatic coupling vectors within linear response time-dependent density functional theory. *Journal of Chemical Physics*, **2009**, 130, 124107	3.9	102
102	Combined QM/MM and classical molecular dynamics study of [Ru(bpy)3]2+ in water. *Journal of Physical Chemistry B*, **2009**, 113, 7737-44	3.4	57

101	Accurate DFT Descriptions for Weak Interactions of Molecules Containing Sulfur. *Journal of Chemical Theory and Computation*, **2009**, 5, 23-8	6.4	35
100	Describing weak interactions of biomolecules with dispersion-corrected density functional theory. *Physical Chemistry Chemical Physics*, **2008**, 10, 2730-4	3.6	56
99	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
98	Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. *Journal of Chemical Physics*, **2008**, 129, 124108	3.9	165
97	DNA structural distortions induced by ruthenium-arene anticancer compounds. *Journal of the American Chemical Society*, **2008**, 130, 10921-8	16.4	88
96	Atom-Centered Potentials to Describe Dispersion Forces in Density Functional Theory. *Chimia*, **2008**, 62, 231-234	1.3	7
95	Copper binding sites in the C-terminal domain of mouse prion protein: A hybrid (QM/MM) molecular dynamics study. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1084-98	4.2	20
94	Parameterization of azole-bridged dinuclear platinum anticancer drugs via a QM/MM force matching procedure. *Journal of Computational Chemistry*, **2008**, 29, 38-49	3.5	30
93	Predicting noncovalent interactions between aromatic biomolecules with London-dispersion-corrected DFT. *Journal of Physical Chemistry B*, **2007**, 111, 14346-54	3.4	61
92	Optical spectra of Cu(II)-azurin by hybrid TDDFT-molecular dynamics simulations. *Journal of Physical Chemistry B*, **2007**, 111, 10248-52	3.4	36
91	Structural and Energetic Properties of Organometallic Ruthenium(II) Diamine Anticancer Compounds and Their Interaction with Nucleobases. *Journal of Chemical Theory and Computation*, **2007**, 3, 1212-22	6.4	24
90	Weakly Bonded Complexes of Aliphatic and Aromatic Carbon Compounds Described with Dispersion Corrected Density Functional Theory. *Journal of Chemical Theory and Computation*, **2007**, 3, 1673-9	6.4	64
89	Protonation of the chromophore in the photoactive yellow protein. *Journal of Physical Chemistry B*, **2007**, 111, 3765-73	3.4	16
88	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, 2315-24	2.9	32
87	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
86	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	3.9	17
85	Trajectory surface hopping within linear response time-dependent density-functional theory. *Physical Review Letters*, **2007**, 98, 023001	7.4	303
84	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

83	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
82	NMR solvent shifts of adenine in aqueous solution from hybrid QM/MM molecular dynamics simulations. *Journal of Physical Chemistry B*, **2007**, 111, 5225-32	3.4	33
81	A comparative theoretical study of dipeptide solvation in water. *Journal of Computational Chemistry*, **2006**, 27, 672-84	3.5	35
80	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
79	Microsolvation effects on the excited-state dynamics of protonated tryptophan. *Journal of the American Chemical Society*, **2006**, 128, 16938-43	16.4	130
78	Duocarmycins binding to DNA investigated by molecular simulation. *Journal of Physical Chemistry B*, **2006**, 110, 3647-60	3.4	25
77	Influence of Hydrogen-Bonding Substituents on the Cytotoxicity of RAPTA Compounds. *Organometallics*, **2006**, 25, 756-765	3.8	148
76	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, 246-50	6.4	26
75	Enantioselective Palladium-Catalyzed Hydrosilylation of Styrene: Influence of Electronic and Steric Effects on Enantioselectivity and Catalyst Design via Hybrid QM/MM Molecular Dynamics Simulations. *Organometallics*, **2006**, 25, 1151-1157	3.8	23
74	Polarization effects and charge transfer in the KcsA potassium channel. *Biophysical Chemistry*, **2006**, 124, 292-301	3.5	78
73	Evolutionarily conserved functional mechanics across pepsin-like and retroviral aspartic proteases. *Journal of the American Chemical Society*, **2005**, 127, 3734-42	16.4	71
72	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
71	Scanning Reactive Pathways with Orbital Biased Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2005**, 1, 554-60	6.4	8
70	Molecular dynamics in electronically excited states using time-dependent density functional theory. *Molecular Physics*, **2005**, 103, 963-981	1.7	120
69	Variational particle number approach for rational compound design. *Physical Review Letters*, **2005**, 95, 153002	7.4	103
68	Hydroxide and proton migration in aquaporins. *Biophysical Journal*, **2005**, 89, 1744-59	2.9	47
67	Solvent and protein effects on the structure and dynamics of the rhodopsin chromophore. *ChemPhysChem*, **2005**, 6, 1836-47	3.2	62
66	Folding pathways for initiator and effector procaspases from computer simulations. *Proteins: Structure, Function and Bioinformatics*, **2005**, 59, 765-72	4.2	4

65	Advances in Density-functional-based Modeling Techniques Recent Extensions of the Car-Parrinello Approach. *Methods and Principles in Medicinal Chemistry*, **2005**, 3-39	0.4	
64	QM/MM Simulation of the First Step of Vision **2005**, 237-243		
63	Quantum Mechanical/Molecular Mechanical (QM/MM) Car-Parrinello Simulations in Excited States. *Chimia*, **2005**, 59, 493-498	1.3	31
62	Rational Design of Organo-Ruthenium Anticancer Compounds. *Chimia*, **2005**, 59, 81-84	1.3	29
61	Variational optimization of effective atom centered potentials for molecular properties. *Journal of Chemical Physics*, **2005**, 122, 14113	3.9	104
60	A molecular spring for vision. *Journal of the American Chemical Society*, **2004**, 126, 15328-9	16.4	88
59	Molecular dynamics simulations of structural changes during procaspase 3 activation. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 932-41	4.2	6
58	Green oxidation catalysts: computational design of high-efficiency models of galactose oxidase. *Angewandte Chemie - International Edition*, **2004**, 43, 3286-9	16.4	24
57	Enantioselective Palladium-Catalyzed Hydrosilylation of Styrene: Detailed Reaction Mechanism from First-Principles and Hybrid QM/MM Molecular Dynamics Simulations. *Organometallics*, **2004**, 23, 3218-3227	3.8	29
56	A Variational Definition of Electrostatic Potential Derived Charges. *Journal of Physical Chemistry B*, **2004**, 108, 7963-7968	3.4	39
55	Unusual Ar-H/Rh-H J(HH) NMR coupling in complexes of rhodium(III): experimental evidence and theoretical support for an eta1-arene structure. *Journal of the American Chemical Society*, **2004**, 126, 12492-502	16.4	26
54	Water-assisted reaction mechanism of monozinc beta-lactamases. *Journal of the American Chemical Society*, **2004**, 126, 12661-8	16.4	92
53	Nuclear Magnetic Resonance Chemical Shifts from Hybrid DFT QM/MM Calculations. *Journal of Physical Chemistry B*, **2004**, 108, 2807-2815	3.4	52
52	Cisplatin Binding to DNA Oligomers from Hybrid Car-Parrinello/Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 2699-2707	3.4	101
51	Theoretical Studies of the Reductive C Bond Cleavage in Complexes of the Form [M(9S3)2]2+ (M = Re, Tc, and Ru; 9S3 = 1,4,7-Trithiacyclononane). *Journal of Physical Chemistry A*, **2004**, 108, 11494-11499	2.8	15
50	First-Principles Simulations of C Bond Cleavage in Rhenium Thioether Complexes. *Journal of Physical Chemistry A*, **2004**, 108, 2008-2013	2.8	18
49	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
48	Optimization of effective atom centered potentials for london dispersion forces in density functional theory. *Physical Review Letters*, **2004**, 93, 153004	7.4	463

47	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
46	Oxidation of Nitrite by Peroxynitrous Acid. *Journal of Physical Chemistry A*, **2003**, 107, 1763-1769	2.8	29
45	Structure-based thermodynamic analysis of caspases reveals key residues for dimerization and activity. *Biochemistry*, **2003**, 42, 8720-8	3.2	15
44	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	3.4	40
43	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
42	Protonation states of methionine aminopeptidase and their relevance for inhibitor binding and catalytic activity. *Journal of Biological Chemistry*, **2003**, 278, 47862-7	5.4	12
41	Drug resistance in HIV-1 protease: Flexibility-assisted mechanism of compensatory mutations. *Protein Science*, **2002**, 11, 2393-402	6.3	105
40	Hybrid Car-Parrinello/Molecular Mechanics Modelling of Transition Metal Complexes: Structure, Dynamics and Reactivity. *QSAR and Combinatorial Science*, **2002**, 21, 119-127		13
39	Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions. *Chimia*, **2002**, 56, 13-19	1.3	53
38	Dialkyl Effect on Enantioselectivity: Stacking as a Structural Feature in P,N Complexes of Palladium(II). *Organometallics*, **2002**, 21, 3033-3041	3.8	35
37	Multiple Steering Molecular Dynamics Applied to Water Exchange at Alkali Ions. *Journal of Physical Chemistry B*, **2002**, 106, 13027-13032	3.4	15
36	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
35	Accelerating rare reactive events by means of a finite electronic temperature. *Journal of the American Chemical Society*, **2002**, 124, 8163-71	16.4	19
34	Canonical Adiabatic Free Energy Sampling (CAFES): A Novel Method for the Exploration of Free Energy Surfaces. *Journal of Physical Chemistry B*, **2002**, 106, 203-208	3.4	68
33	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
32	A Hamiltonian electrostatic coupling scheme for hybrid Car-Parrinello molecular dynamics simulations. *Journal of Chemical Physics*, **2002**, 116, 6941-6947	3.9	540
31	Early steps of the intramolecular signal transduction in rhodopsin explored by molecular dynamics simulations. *Biochemistry*, **2002**, 41, 10799-809	3.2	102
30	15 Years of Car-Parrinello Simulations in Physics, Chemistry and Biology. *Computational Chemistry - Reviews of Current Trends*, **2001**, 33-68		9

29	Estimating equilibrium properties from non-Hamiltonian dynamics. *Journal of Chemical Physics*, **2001**, 115, 7859-7864	3.9	2
28	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
27	Cis-trans isomerization in triply-bonded ditungsten complexes: a multitude of possible pathways. *Inorganic Chemistry*, **2001**, 40, 5780-6	5.1	6
26	Isolation of a Highly Persistent Diphosphanyl Radical: The Phosphorus Analogue of a Hydrazyl This work was supported by the ETH Zürich and Swiss National Science Foundation.. *Angewandte Chemie - International Edition*, **2001**, 40, 723-726	16.4	2
25	Efficient multidimensional free energy calculations for ab initio molecular dynamics using classical bias potentials. *Journal of Chemical Physics*, **2000**, 113, 4863	3.9	27
24	Three- and four-center trans effects in triply bonded ditungsten complexes: an ab initio molecular dynamics study of compounds with stoichiometry W2Cl4(NHEt)2(PMe3)2. *Inorganic Chemistry*, **2000**, 39, 5553-60	5.1	12
23	Ditantalum Hydride Complexes with Bridging (2,6-iPr2C6H3)NSiHPh Silanimine Ligands Resulting from PhSiH3 Imido Ligand Coupling. A Combined Spectroscopic and Theoretical Investigation. *Organometallics*, **2000**, 19, 3830-3841	3.8	39
22	Chiral Palladium(II) Bis(trichlorosilyl) Complexes. Synthesis, Structure, and Combined QM/MM Computational Studies. *Organometallics*, **2000**, 19, 2144-2152	3.8	31
21	Conformational Equilibria of Peroxynitrous Acid in Water: A First-Principles Molecular Dynamics Study. *Journal of Physical Chemistry A*, **2000**, 104, 6464-6469	2.8	22
20	Electronically and Sterically Induced Structural Distortions in Square-Planar d8 Complexes. *Organometallics*, **2000**, 19, 3591-3596	3.8	19
19	Conformational and orientational order and disorder in solid polytetrafluoroethylene. *Molecular Physics*, **1999**, 97, 355-373	1.7	35
18	Ab initio molecular dynamics studies of a synthetic biomimetic model of galactose oxidase. *International Journal of Quantum Chemistry*, **1999**, 73, 209-218	2.1	30
17	Ab initio molecular dynamics simulations of the gas-phase reaction of hydroxyl radical with nitrogen dioxide radical. *Chemical Physics Letters*, **1998**, 297, 205-210	2.5	25
16	Living polymers. *Journal of the Chemical Society, Faraday Transactions*, **1998**, 94, 501-508		20
15	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	0.4	4
14	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. *Journal of Chemical Physics*, **1997**, 106, 4658-4664	3.9	87
13	Structure of Solid Poly(tetrafluoroethylene): A Computer Simulation Study of Chain Orientational, Translational, and Conformational Disorder. *Journal of Physical Chemistry B*, **1997**, 101, 2745-2749	3.4	37
12	The torsional potential of perfluoro n-alkanes: A density functional study. *Journal of Chemical Physics*, **1996**, 104, 3692-3700	3.9	48

11	Na6Pb: a bimetallic cluster of striking stability. *Chemical Physics Letters*, **1995**, 237, 334-338	2.5	36
10	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	2.5	21
9	Structure of nanoscale silicon clusters. *Physical Review Letters*, **1994**, 72, 665-668	7.4	262
8	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		7
7	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
6	Metal clusters with impurities: NanMg (n=6□, 18). *Chemical Physics Letters*, **1992**, 198, 478-482	2.5	26
5	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
4	Sodium cluster ionisation potentials revisited: Higher-resolution measurements for Nax (x. *Chemical Physics Letters*, **1988**, 143, 251-258	2.5	187
3	On the accuracy of molecular simulation-based predictions of koff values: a Metadynamics study		1
2	Regulation of adenylyl cyclase 5 in striatal neurons confers the ability to detect coincident neuromodulatory signals		1
1	Methylammonium Triiodide for Defect Engineering of High-Efficiency Perovskite Solar Cells. *ACS Energy Letters*,3650-3660	20.1	8