# Ursula RÃ¶thlisberger

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | 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 |
| 2 | Recent Advances in First-Principles Based Molecular Dynamics. Accounts of Chemical Research, 2022, 55, 221-230. | 7.6 | 22 |
| 3 | A universal co-solvent dilution strategy enables facile and cost-effective fabrication of perovskite photovoltaics. Nature Communications, 2022, 13, 89. | 5.8 | 77 |
| 4 | A multiple time step algorithm for trajectory surface hopping simulations. Journal of Chemical Physics, 2022, 156, 034107. | 1.2 | 2 |
| 5 | A theoretical perspective of the ultrafast transient absorption dynamics of <scp>CsPbBr<sub>3</sub></scp>. Journal of Computational Chemistry, 2022, 43, 577-582. | 1.5 | 3 |
| 6 | Reversible Pressureâ€Dependent Mechanochromism of Dionâ€“Jacobson and Ruddlesdenâ€“Popper Layered Hybrid Perovskites. Advanced Materials, 2022, 34, e2108720. | 11.1 | 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. | 3.2 | 3 |
| 8 | Wavefunction-Based Electrostatic-Embedding QM/MM Using CFOUR through MiMiC. Journal of Chemical Theory and Computation, 2022, 18, 13-24. | 2.3 | 2 |
| 9 | Kinetics and energeticsÂof metal halide perovskite conversion reactions at the nanoscale. Communications Materials, 2022, 3, . | 2.9 | 12 |
| 10 | GÎ±i1 inhibition mechanism of ATP-bound adenylyl cyclase type 5. PLoS ONE, 2021, 16, e0245197. | 1.1 | 5 |
| 11 | Molecular Origin of the Asymmetric Photoluminescence Spectra of CsPbBr<sub>3</sub> at Low Temperature. Journal of Physical Chemistry Letters, 2021, 12, 2699-2704. | 2.1 | 12 |
| 12 | Pseudo-halide anion engineering for Î±-FAPbI3 perovskite solar cells. Nature, 2021, 592, 381-385. | 13.7 | 2,095 |
| 13 | A combined molecular dynamics and experimental study of two-step process enabling low-temperature formation of phase-pure Î±-FAPbI <sub>3</sub>. Science Advances, 2021, 7, . | 4.7 | 49 |
| 14 | Ultrafast pulse shaping modulates perceived visual brightness in living animals. Science Advances, 2021, 7, . | 4.7 | 2 |
| 15 | Expanding the boundaries of ligandâ€“target modeling by exascale calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1535. | 6.2 | 13 |
| 16 | Organic Spacers in 2D Perovskites: General Trends and Structureâ€Property Relationships from Computational Studies. Helvetica Chimica Acta, 2021, 104, e2000232. | 1.0 | 6 |
| 17 | Multimodal hostâ€“guest complexation for efficient and stable perovskite photovoltaics. Nature Communications, 2021, 12, 3383. | 5.8 | 72 |
| 18 | Naphthalenediimide/Formamidinium-Based Low-Dimensional Perovskites. Chemistry of Materials, 2021, 33, 6412-6420. | 3.2 | 16 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Methylammonium Triiodide for Defect Engineering of High-Efficiency Perovskite Solar Cells. ACS Energy Letters, 2021, 6, 3650-3660. | 8.8 | 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. | 6.6 | 55 |
| 21 | Nanoscale interfacial engineering enables highly stable and efficient perovskite photovoltaics. Energy and Environmental Science, 2021, 14, 5552-5562. | 15.6 | 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. | 3.0 | 5 |
| 23 | Atomistic Mechanism of the Nucleation of Methylammonium Lead Iodide Perovskite from Solution. Chemistry of Materials, 2020, 32, 529-536. | 3.2 | 45 |
| 24 | Guanineâ€Stabilized Formamidinium Lead Iodide Perovskites. Angewandte Chemie - International Edition, 2020, 59, 4691-4697. | 7.2 | 61 |
| 25 | Guanineâ€Stabilized Formamidinium Lead Iodide Perovskites. Angewandte Chemie, 2020, 132, 4721-4727. | 1.6 | 0 |
| 26 | Accuracy of Molecular Simulation-Based Predictions of k<sub>off</sub> Values: A Metadynamics Study. Journal of Physical Chemistry Letters, 2020, 11, 6373-6381. | 2.1 | 41 |
| 27 | Formamidiniumâ€Based Dionâ€Jacobson Layered Hybrid Perovskites: Structural Complexity and Optoelectronic Properties. Advanced Functional Materials, 2020, 30, 2003428. | 7.8 | 61 |
| 28 | Structural and Photophysical Templating of Conjugated Polyelectrolytes with Single-Stranded DNA. Chemistry of Materials, 2020, 32, 7347-7362. | 3.2 | 4 |
| 29 | 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 |
| 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. | 2.3 | 15 |
| 31 | Multidisciplinary Preclinical Investigations on Three Oxamniquine Analogues as New Drug Candidates for Schistosomiasis**. Chemistry - A European Journal, 2020, 26, 15232-15241. | 1.7 | 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. | 1.3 | 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. | 2.3 | 2 |
| 34 | Crown Ether Modulation Enables over 23% Efficient Formamidinium-Based Perovskite Solar Cells. Journal of the American Chemical Society, 2020, 142, 19980-19991. | 6.6 | 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. | 10.8 | 56 |
| 36 | Atomistic Origins of the Limited Phase Stability of Cs<sup>+</sup>-Rich FA<sub>x</sub>Cs<sub>(1â€“x)</sub>PbI<sub>3</sub> Mixtures. Chemistry of Materials, 2020, 32, 2605-2614. | 3.2 | 24 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | MiMiC: Multiscale Modeling in Computational Chemistry. Frontiers in Molecular Biosciences, 2020, 7, 45. | 1.6 | 5 |
| 38 | Molecular Basis of CLC Antiporter Inhibition by Fluoride. Journal of the American Chemical Society, 2020, 142, 7254-7258. | 6.6 | 20 |
| 39 | Vapor-assisted deposition of highly efficient, stable black-phase FAPbI <sub>3</sub> perovskite solar cells. Science, 2020, 370, . | 6.0 | 530 |
| 40 | Biomolecular Simulation: A Perspective from High Performance Computing. Israel Journal of Chemistry, 2020, 60, 694-704. | 1.0 | 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. | 6.6 | 104 |
| 42 | 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 |
| 43 | Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. Journal of Chemical Theory and Computation, 2019, 15, 5601-5613. | 2.3 | 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. | 1.3 | 3 |
| 45 | Association of Both Inhibitory and Stimulatory GÎ± Subunits Implies Adenylyl Cyclase 5 Deactivation. Biochemistry, 2019, 58, 4317-4324. | 1.2 | 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. | 2.3 | 19 |
| 47 | Ruddlesdenâ€“Popper Phases of Methylammonium-Based Two-Dimensional Perovskites with 5-Ammonium Valeric Acid AVA<sub>2</sub>MA<sub>nâ€“1</sub>Pb<sub>n</sub>I<sub>3n+1</sub> with n = 1, 2, and 3. Journal of Physical Chemistry Letters, 2019, 10, 3543-3549. | 2.1 | 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. | 5.5 | 76 |
| 49 | MiMiC: A Novel Framework for Multiscale Modeling in Computational Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 3810-3823. | 2.3 | 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. | 2.3 | 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. | 5.0 | 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. | 2.3 | 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. | 2.3 | 24 |
| 54 | The Structure of the Protonated Serine Octamer. Journal of the American Chemical Society, 2018, 140, 7554-7560. | 6.6 | 67 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | 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 |
| 56 | Exploiting Coordinate Scaling Relations To Accelerate Exact Exchange Calculations. Journal of Physical Chemistry Letters, 2018, 9, 3886-3890. | 2.1 | 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. | 3.3 | 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, . | 2.1 | 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. | 2.1 | 114 |
| 60 | Allosteric cross-talk in chromatin can mediate drug-drug synergy. Nature Communications, 2017, 8, 14860. | 5.8 | 61 |
| 61 | Development of Site-Specific Mg<sup>2+</sup>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 |
| 62 | Effect of N-Terminal Myristoylation on the Active Conformation of GÎ±<sub>i1</sub>â€“GTP. Biochemistry, 2017, 56, 271-280. | 1.2 | 18 |
| 63 | Predictive Determination of Band Gaps of Inorganic Halide Perovskites. Journal of Physical Chemistry Letters, 2017, 8, 5507-5512. | 2.1 | 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. | 2.3 | 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. | 1.5 | 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. | 2.3 | 10 |
| 67 | Does Proton Conduction in the Voltage-Gated H<sup>+</sup> Channel hHv1 Involve Grotthuss-Like Hopping via Acidic Residues?. Journal of Physical Chemistry B, 2017, 121, 3340-3351. | 1.2 | 34 |
| 68 | Nonadiabatic effects in electronic and nuclear dynamics. Structural Dynamics, 2017, 4, 061510. | 0.9 | 31 |
| 69 | Charge migration and charge transfer in molecular systems. Structural Dynamics, 2017, 4, 061508. | 0.9 | 146 |
| 70 | 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 |
| 71 | Charge separation and carrier dynamics in donor-acceptor heterojunction photovoltaic systems. Structural Dynamics, 2017, 4, 061503. | 0.9 | 13 |
| 72 | Implications of short time scale dynamics on long time processes. Structural Dynamics, 2017, 4, 061507. | 0.9 | 24 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Exploring the inhibition mechanism of adenylyl cyclase type 5 by n-terminal myristoylated GÎ±i1. PLoS Computational Biology, 2017, 13, e1005673. | 1.5 | 17 |
| 74 | An Organometallic Compound which Exhibits a DNA Topologyâ€Dependent Oneâ€Stranded Intercalation Mode. Angewandte Chemie, 2016, 128, 7567-7570. | 1.6 | 0 |
| 75 | Molecular Mechanism of Chromatin Targeting by a Potent Anticancer Agent Acting at the Nucleosome Core Particle. Biophysical Journal, 2016, 110, 68a-69a. | 0.2 | 0 |
| 76 | Ultrafast Relaxation Dynamics of the Ethylene Cation C<sub>2</sub>H<sub>4</sub><sup>+</sup>. Journal of Physical Chemistry Letters, 2016, 7, 1901-1906. | 2.1 | 23 |
| 77 | Geneticâ€Algorithmâ€Based Optimization of a Peptidic Scaffold for Sequestration and Hydration of CO<sub>2</sub>. ChemPhysChem, 2016, 17, 3831-3835. | 1.0 | 3 |
| 78 | Extended Intermolecular Interactions Governing Photocurrentâ€“Voltage Relations in Ternary Organic Solar Cells. Journal of Physical Chemistry Letters, 2016, 7, 3936-3944. | 2.1 | 11 |
| 79 | Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies. ChemMedChem, 2016, 11, 1199-1210. | 1.6 | 104 |
| 80 | Valence and conduction band tuning in halide perovskites for solar cell applications. Journal of Materials Chemistry A, 2016, 4, 15997-16002. | 5.2 | 132 |
| 81 | Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. Science Advances, 2016, 2, e1601156. | 4.7 | 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. | 6.6 | 79 |
| 83 | An Organometallic Compound which Exhibits a DNA Topologyâ€Dependent Oneâ€Stranded Intercalation Mode. Angewandte Chemie - International Edition, 2016, 55, 7441-7444. | 7.2 | 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. | 5.2 | 47 |
| 85 | Ionic polarization-induced currentâ€“voltage hysteresis in CH3NH3PbX3 perovskite solar cells. Nature Communications, 2016, 7, 10334. | 5.8 | 602 |
| 86 | Entropic stabilization of mixed A-cation ABX<sub>3</sub> metal halide perovskites for high performance perovskite solar cells. Energy and Environmental Science, 2016, 9, 656-662. | 15.6 | 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. | 1.2 | 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. | 2.1 | 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. | 23.0 | 352 |
| 90 | In Situ Mapping of the Molecular Arrangement of Amphiphilic Dye Molecules at the TiO<sub>2</sub> Surface of Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 10834-10842. | 4.0 | 30 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. Journal of the American Chemical Society, 2015, 137, 11170-11178. | 6.6 | 86 |
| 92 | Local Control Theory in Trajectory Surface Hopping Dynamics Applied to the Excitedâ€Šstate Proton Transfer of 4â€²Hydroxyacridine. ChemPhysChem, 2015, 16, 2127-2133. | 1.0 | 9 |
| 93 | Computational insights into function and inhibition of fatty acid amide hydrolase. European Journal of Medicinal Chemistry, 2015, 91, 15-26. | 2.6 | 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. | 1.5 | 31 |
| 95 | Study of the Redox Properties of Singlet and Triplet Tris(2,2â€²-bipyridine)ruthenium(II) ([Ru(bpy)<sub>3</sub>]<sup>2+</sup>) 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 |
| 96 | Lessons from Nature: Computational Design of Biomimetic Compounds and Processes. Chimia, 2014, 68, 642. | 0.3 | 4 |
| 97 | Ligand substitutions between rutheniumâ€“cymene compounds can control protein versus DNA targeting and anticancer activity. Nature Communications, 2014, 5, 3462. | 5.8 | 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. | 1.3 | 39 |
| 99 | 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 |
| 100 | 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 |
| 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. | 2.3 | 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. | 1.2 | 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. | 6.6 | 17 |
| 104 | A Vibronic Coupling Hamiltonian to Describe the Ultrafast Excited State Dynamics of a Cu(I)-Phenanthroline Complex. Chimia, 2014, 68, 227. | 0.3 | 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. | 1.0 | 14 |
| 106 | Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454. | 2.3 | 81 |
| 107 | Nonadiabatic ab initio molecular dynamics using linear-response time-dependent density functional theory. Open Physics, 2013, 11, . | 0.8 | 6 |
| 108 | Photodynamics of Lys+-Trp protein motifs: Hydrogen bonds ensure photostability. Faraday Discussions, 2013, 163, 189. | 1.6 | 7 |

| # | ARTICLE | IF | CITATIONS |
|---|---|---|---|
| 109 | In situparameterisation of SCC-DFTB repulsive potentials by iterative Boltzmann inversion. Molecular Physics, 2013, 111, 3595-3607. | 0.8 | 28 |
| 110 | Wagging the Tail: Essential Role of Substrate Flexibility in FAAH Catalysis. Journal of Chemical Theory and Computation, 2013, 9, 1202-1213. | 2.3 | 24 |
| 111 | Intricacies of Describing Weak Interactions Involving Halogen Atoms within Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 955-964. | 2.3 | 24 |
| 112 | Charge transfer relaxation in donorâ€“acceptor type conjugated materials. Journal of Materials Chemistry C, 2013, 1, 2308. | 2.7 | 54 |
| 113 | Mechanism to Trigger Unfolding in O<sup>6</sup>â€Alkylguanineâ€DNA Alkyltransferase. ChemBioChem, 2013, 14, 703-710. | 1.3 | 7 |
| 114 | Trajectoryâ€Based Nonadiabatic Dynamics with Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2013, 14, 1314-1340. | 1.0 | 168 |
| 115 | Molecular Engineering of a Fluorene Donor for Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2733-2739. | 3.2 | 154 |
| 116 | Unravelling the Potential for Dithienopyrrole Sensitizers in Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2642-2648. | 3.2 | 49 |
| 117 | Two Misfolding Routes for the Prion Protein around pH 4.5. PLoS Computational Biology, 2013, 9, e1003057. | 1.5 | 18 |
| 118 | Local Control Theory using Trajectory Surface Hopping and Linear-Response Time-Dependent Density Functional Theory. Chimia, 2013, 67, 218-221. | 0.3 | 6 |
| 119 | Ultrafast anisotropic x-ray scattering in the condensed phase. New Journal of Physics, 2012, 14, 113002. | 1.2 | 11 |
| 120 | Excited State Dynamics with Quantum Trajectories. Chimia, 2012, 66, 174. | 0.3 | 5 |
| 121 | Directed Evolution of the Suicide Protein O<sup>6</sup>-Alkylguanine-DNA Alkyltransferase for Increased Reactivity Results in an Alkylated Protein with Exceptional Stability. Biochemistry, 2012, 51, 986-994. | 1.2 | 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. | 6.6 | 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. | 1.9 | 165 |
| 124 | Simulations of X-ray absorption spectra: the effect of the solvent. Physical Chemistry Chemical Physics, 2012, 14, 9444. | 1.3 | 25 |
| 125 | Role of Environment for Catalysis of the DNA Repair Enzyme MutY. Journal of the American Chemical Society, 2012, 134, 8608-8616. | 6.6 | 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. | 2.3 | 247 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Nanocomposites Containing Neutral Blue Emitting Cyclometalated Iridium(III) Emitters for Oxygen Sensing. Chemistry of Materials, 2012, 24, 2330-2338. | 3.2 | 63 |
| 128 | Influence of Halogen Atoms on a Homologous Series of Bis-Cyclometalated Iridium(III) Complexes. Inorganic Chemistry, 2012, 51, 799-811. | 1.9 | 107 |
| 129 | A Simple Approach to Room Temperature Phosphorescent Allenylidene Complexes. Angewandte Chemie - International Edition, 2012, 51, 8030-8033. | 7.2 | 20 |
| 130 | Integrating computational methods to retrofit enzymes to synthetic pathways. Biotechnology and Bioengineering, 2012, 109, 572-582. | 1.7 | 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. | 2.3 | 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. | 1.3 | 64 |
| 133 | Identification of clustering artifacts in photoactivated localization microscopy. Nature Methods, 2011, 8, 527-528. | 9.0 | 197 |
| 134 | Secondary Structure Assignment of Amyloid-Î² Peptide Using Chemical Shifts. Journal of Chemical Theory and Computation, 2011, 7, 1552-1563. | 2.3 | 14 |
| 135 | Quantitative Photo Activated Localization Microscopy: Unraveling the Effects of Photoblinking. PLoS ONE, 2011, 6, e22678. | 1.1 | 252 |
| 136 | Mechanical (QM/MM) Simulations of Adiabatic and Nonadiabatic Ultrafast Phenomena. Chimia, 2011, 65, 330-333. | 0.3 | 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. | 0.9 | 101 |
| 138 | Coldâ€Ion Spectroscopy Reveals the Intrinsic Structure of a Decapeptide. Angewandte Chemie - International Edition, 2011, 50, 5383-5386. | 7.2 | 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. | 1.7 | 73 |
| 140 | Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems. Chimia, 2011, 65, 667. | 0.3 | 22 |
| 141 | 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 |
| 142 | Electron Localization Dynamics in the Triplet Excited State of [Ru(bpy)<sub>3</sub>]<sup>2+</sup> in Aqueous Solution. Chemistry - A European Journal, 2010, 16, 5889-5894. | 1.7 | 68 |
| 143 | Reactions of Alkynes with [RuCl(cyclopentadienyl)] Complexes: The Important First Steps. Chemistry - A European Journal, 2010, 16, 8400-8409. | 1.7 | 50 |
| 144 | Molecular simulations of ion channels: a quantum chemistâ€™s perspective. Journal of General Physiology, 2010, 135, 549-554. | 0.9 | 35 |

| # | Article | IF | Citations |
|---|---|---|---|
| 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. | 1.2 | 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. | 2.3 | 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. | 0.2 | 64 |
| 148 | Mixed quantum-classical dynamics with time-dependent external fields: A time-dependent density-functional-theory approach. Physical Review A, 2010, 81, . | 1.0 | 49 |
| 149 | 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 |
| 150 | On nonadiabatic coupling vectors in time-dependent density functional theory. Journal of Chemical Physics, 2009, 131, 196101. | 1.2 | 80 |
| 151 | A QM/MM Investigation of Thymine Dimer Radical Anion Splitting Catalyzed by DNA Photolyase. ChemPhysChem, 2009, 10, 400-410. | 1.0 | 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. | 1.2 | 60 |
| 154 | Developing Improved Charge Sets for the Modeling of the KcsA K<sup>+</sup> Channel Using QM/MM Electrostatic Potentials. Journal of Chemical Theory and Computation, 2009, 5, 2173-2179. | 2.3 | 17 |
| 155 | Tuning the Efficacy of Ruthenium(II)-Arene (RAPTA) Antitumor Compounds with Fluorinated Arene Ligands. Organometallics, 2009, 28, 5061-5071. | 1.1 | 61 |
| 156 | Dispersion Corrected Atom-Centered Potentials for Phosphorus. Journal of Chemical Theory and Computation, 2009, 5, 2930-2934. | 2.3 | 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. | 1.1 | 21 |
| 158 | New Paradigm in Molecular Engineering of Sensitizers for Solar Cell Applications. Journal of the American Chemical Society, 2009, 131, 5930-5934. | 6.6 | 385 |
| 159 | Importance of van der Waals Interactions in Liquid Water. Journal of Physical Chemistry B, 2009, 113, 1127-1131. | 1.2 | 175 |
| 160 | Drug resistance in HIV-1 protease: Flexibility-assisted mechanism of compensatory mutations. Protein Science, 2009, 11, 2393-2402. | 3.1 | 124 |
| 161 | Binding of Organometallic Ruthenium(II) Anticancer Compounds to Nucleobases: A Computational Study. Journal of Physical Chemistry A, 2009, 113, 11888-11897. | 1.1 | 34 |
| 162 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 163 | Nonadiabatic coupling vectors within linear response time-dependent density functional theory. Journal of Chemical Physics, 2009, 130, 124107. | 1.2 | 114 |
| 164 | Combined QM/MM and Classical Molecular Dynamics Study of [Ru(bpy)<sub>3</sub>]<sup>2+</sup> in Water. Journal of Physical Chemistry B, 2009, 113, 7737-7744. | 1.2 | 61 |
| 165 | Accurate DFT Descriptions for Weak Interactions of Molecules Containing Sulfur. Journal of Chemical Theory and Computation, 2009, 5, 23-28. | 2.3 | 38 |
| 166 | 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 |
| 167 | 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 |
| 168 | Describing weak interactions of biomolecules with dispersion-corrected density functional theory. Physical Chemistry Chemical Physics, 2008, 10, 2730. | 1.3 | 59 |
| 169 | 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 |
| 170 | Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. Journal of Chemical Physics, 2008, 129, 124108. | 1.2 | 182 |
| 171 | DNA Structural Distortions Induced by Rutheniumâ^'Arene Anticancer Compounds. Journal of the American Chemical Society, 2008, 130, 10921-10928. | 6.6 | 94 |
| 172 | Atom-Centered Potentials to Describe Dispersion Forces in Density Functional Theory. Chimia, 2008, 62, 231. | 0.3 | 7 |
| 173 | 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 |
| 174 | Trajectory Surface Hopping within Linear Response Time-Dependent Density-Functional Theory. Physical Review Letters, 2007, 98, 023001. | 2.9 | 324 |
| 175 | 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 |
| 176 | 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 |
| 177 | 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 |
| 178 | Predicting Noncovalent Interactions between Aromatic Biomolecules with London-Dispersion-Corrected DFT. Journal of Physical Chemistry B, 2007, 111, 14346-14354. | 1.2 | 62 |
| 179 | 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 |
| 180 | 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 |

| # | ARTICLE | IF | CITATIONS |
|---|---|---|---|
| 181 | 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 |
| 182 | Protonation of the Chromophore in the Photoactive Yellow Protein. Journal of Physical Chemistry B, 2007, 111, 3765-3773. | 1.2 | 17 |
| 183 | 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 |
| 184 | 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 |
| 185 | Microsolvation Effects on the Excited-State Dynamics of Protonated Tryptophan. Journal of the American Chemical Society, 2006, 128, 16938-16943. | 6.6 | 144 |
| 186 | Duocarmycins Binding to DNA Investigated by Molecular Simulationâ€. Journal of Physical Chemistry B, 2006, 110, 3647-3660. | 1.2 | 26 |
| 187 | Influence of Hydrogen-Bonding Substituents on the Cytotoxicity of RAPTA Compounds. Organometallics, 2006, 25, 756-765. | 1.1 | 154 |
| 188 | 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 |
| 189 | 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 |
| 190 | Polarization effects and charge transfer in the KcsA potassium channel. Biophysical Chemistry, 2006, 124, 292-301. | 1.5 | 84 |
| 191 | A comparative theoretical study of dipeptide solvation in water. Journal of Computational Chemistry, 2006, 27, 672-684. | 1.5 | 37 |
| 192 | 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 |
| 193 | Solvent and Protein Effects on the Structure and Dynamics of the Rhodopsin Chromophore. ChemPhysChem, 2005, 6, 1836-1847. | 1.0 | 65 |
| 194 | Folding pathways for initiator and effector procaspases from computer simulations. Proteins: Structure, Function and Bioinformatics, 2005, 59, 765-772. | 1.5 | 4 |
| 195 | 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 |
| 196 | QM/MM Simulation of the First Step of Vision. , 2005, , 237-243. | | 0 |
| 197 | Quantum Mechanical/Molecular Mechanical (QM/MM) Car-Parrinello Simulations in Excited States. Chimia, 2005, 59, 493-498. | 0.3 | 34 |
| 198 | Rational Design of Organo-Ruthenium Anticancer Compounds. Chimia, 2005, 59, 81-84. | 0.3 | 33 |

| # | ARTICLE | IF | CITATIONS |
|---|---|---|---|
| 199 | Variational optimization of effective atom centered potentials for molecular properties. Journal of Chemical Physics, 2005, 122, 014113. | 1.2 | 110 |
| 200 | Evolutionarily Conserved Functional Mechanics across Pepsin-like and Retroviral Aspartic Proteases. Journal of the American Chemical Society, 2005, 127, 3734-3742. | 6.6 | 74 |
| 201 | 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 |
| 202 | Scanning Reactive Pathways with Orbital Biased Molecular Dynamics. Journal of Chemical Theory and Computation, 2005, 1, 554-560. | 2.3 | 8 |
| 203 | Molecular dynamics in electronically excited states using time-dependent density functional theory. Molecular Physics, 2005, 103, 963-981. | 0.8 | 130 |
| 204 | Variational Particle Number Approach for Rational Compound Design. Physical Review Letters, 2005, 95, 153002. | 2.9 | 112 |
| 205 | Hydroxide and Proton Migration in Aquaporins. Biophysical Journal, 2005, 89, 1744-1759. | 0.2 | 56 |
| 206 | A Molecular Spring for Vision. Journal of the American Chemical Society, 2004, 126, 15328-15329. | 6.6 | 98 |
| 207 | Molecular dynamics simulations of structural changes during procaspase 3 activation. Proteins: Structure, Function and Bioinformatics, 2004, 55, 932-941. | 1.5 | 6 |
| 208 | Green Oxidation Catalysts: Computational Design of High-Efficiency Models of Galactose Oxidase. Angewandte Chemie - International Edition, 2004, 43, 3286-3289. | 7.2 | 29 |
| 209 | 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 |
| 210 | A Variational Definition of Electrostatic Potential Derived Charges. Journal of Physical Chemistry B, 2004, 108, 7963-7968. | 1.2 | 40 |
| 211 | 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 |
| 212 | Water-Assisted Reaction Mechanism of Monozinc Î²-Lactamases. Journal of the American Chemical Society, 2004, 126, 12661-12668. | 6.6 | 99 |
| 213 | Nuclear Magnetic Resonance Chemical Shifts from Hybrid DFT QM/MM Calculations. Journal of Physical Chemistry B, 2004, 108, 2807-2815. | 1.2 | 58 |
| 214 | Cisplatin Binding to DNA Oligomers from Hybrid Car-Parrinello/Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 2699-2707. | 1.2 | 109 |
| 215 | Theoretical Studies of the Reductive Câ^'S Bond Cleavage in Complexes of the Form [M(9S3)2]2+ (M = Re,) Tj ETQq1 1 0.784314 rgB | 1.1 | 18 |
| 216 | First-Principles Simulations of Câ^'S Bond Cleavage in Rhenium Thioether Complexes. Journal of Physical Chemistry A, 2004, 108, 2008-2013. | 1.1 | 21 |

| # | Article | IF | Citations |
|---|---|---|---|
| 217 | 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 |
| 218 | Optimization of Effective Atom Centered Potentials for London Dispersion Forces in Density Functional Theory. Physical Review Letters, 2004, 93, 153004. | 2.9 | 489 |
| 219 | 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 |
| 220 | Oxidation of Nitrite by Peroxynitrous Acid. Journal of Physical Chemistry A, 2003, 107, 1763-1769. | 1.1 | 29 |
| 221 | Structure-Based Thermodynamic Analysis of Caspases Reveals Key Residues for Dimerization and Activityâ€. Biochemistry, 2003, 42, 8720-8728. | 1.2 | 16 |
| 222 | 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 |
| 223 | 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 |
| 224 | 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 |
| 225 | Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions. Chimia, 2002, 56, 13-19. | 0.3 | 62 |
| 226 | 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 |
| 227 | Multiple Steering Molecular Dynamics Applied to Water Exchange at Alkali Ions. Journal of Physical Chemistry B, 2002, 106, 13027-13032. | 1.2 | 15 |
| 228 | 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 |
| 229 | Accelerating Rare Reactive Events by Means of a Finite Electronic Temperature. Journal of the American Chemical Society, 2002, 124, 8163-8171. | 6.6 | 20 |
| 230 | 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 |
| 231 | 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 |
| 232 | A Hamiltonian electrostatic coupling scheme for hybrid Carâ€“Parrinello molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 6941-6947. | 1.2 | 588 |
| 233 | Early Steps of the Intramolecular Signal Transduction in Rhodopsin Explored by Molecular Dynamics Simulationsâ€. Biochemistry, 2002, 41, 10799-10809. | 1.2 | 111 |
| 234 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 235 | 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 |
| 236 | Cisâ^'TransIsomerization in Triply-Bonded Ditungsten Complexes:Â A Multitude of Possible Pathways. Inorganic Chemistry, 2001, 40, 5780-5786. | 1.9 | 8 |
| 237 | 15 Years of Car-Parrinello Simulations in Physics, Chemistry and Biology. Computational Chemistry - Reviews of Current Trends, 2001, , 33-68. | 0.4 | 10 |
| 238 | Estimating equilibrium properties from non-Hamiltonian dynamics. Journal of Chemical Physics, 2001, 115, 7859-7864. | 1.2 | 2 |
| 239 | 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 |
| 240 | Efficient multidimensional free energy calculations for ab initio molecular dynamics using classical bias potentials. Journal of Chemical Physics, 2000, 113, 4863. | 1.2 | 30 |
| 241 | 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 |
| 242 | 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 |
| 243 | Chiral Palladium(II)â^'Bis(trichlorosilyl) Complexes. Synthesis, Structure, and Combined QM/MM Computational Studies. Organometallics, 2000, 19, 2144-2152. | 1.1 | 33 |
| 244 | 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 |
| 245 | Electronically and Sterically Induced Structural Distortions in Square-Planar d8 Complexes. Organometallics, 2000, 19, 3591-3596. | 1.1 | 20 |
| 246 | Conformational and orientational order and disorder in solid polytetrafluoroethylene. Molecular Physics, 1999, 97, 355-373. | 0.8 | 37 |
| 247 | 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 |
| 248 | 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 |
| 249 | 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 |
| 250 | 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 |
| 251 | Ab initio molecular dynamics simulation of liquid hydrogen fluoride. Journal of Chemical Physics, 1997, 106, 4658-4664. | 1.2 | 95 |
| 252 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 253 | The torsional potential of perfluoronâ€alkanes: A density functional study. Journal of Chemical Physics, 1996, 104, 3692-3700. | 1.2 | 56 |
| 254 | Na6Pb: a bimetallic cluster of striking stability. Chemical Physics Letters, 1995, 237, 334-338. | 1.2 | 40 |
| 255 | 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 |
| 256 | Structure of nanoscale silicon clusters. Physical Review Letters, 1994, 72, 665-668. | 2.9 | 288 |
| 257 | 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 |
| 258 | 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 |
| 259 | Metal clusters with impurities: NanMg (n=6â^’9, 18). Chemical Physics Letters, 1992, 198, 478-482. | 1.2 | 27 |
| 260 | 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 |
| 261 | 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 |
| 262 | Molecular Dynamics Simulations of Nucleation of Lead Halide Perovskites. , 0, , . | | 0 |
| 263 | Molecular Dynamics Simulations of Nucleation of Lead Halide Perovskites. , 0, , . | | 0 |
| 264 | Multiscale molecular simulations to investigate adenylyl cyclaseâ€based signaling in the brain. Wiley Interdisciplinary Reviews: Computational Molecular Science, 0, , . | 6.2 | 2 |
| 265 | Reversible photo de-mixing in two-dimensional Dion-Jacobson mixed halide perovskites: photo-miscibility gap mapped. , 0, , . | | 0 |