# Manuel F Ruiz-LÃ³pez

List of Publications by Year
in descending order



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|---|---|---|---|
| 213 papers | 6,667 citations | 47 h-index | 67 g-index |
| | | 47006 | 98798 |
| 220 all docs | 220 docs citations | 220 times ranked | 5237 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Photosensitization mechanisms at the airâ€“water interface of aqueous aerosols. Chemical Science, 2022, 13, 2624-2631. | 7.4 | 17 |
| 2 | Reactivity of Undissociated Molecular Nitric Acid at the Airâ€“Water Interface. Journal of the American Chemical Society, 2021, 143, 453-462. | 13.7 | 14 |
| 3 | Tight electrostatic regulation of the OH production rate from the photolysis of hydrogen peroxide adsorbed on surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, . | 7.1 | 9 |
| 4 | Mechanistic insights into lysine-targeting covalent inhibition through a theoretical study of ester aminolysis. Organic and Biomolecular Chemistry, 2021, 19, 9996-10004. | 2.8 | 1 |
| 5 | Midair transformations of aerosols. Science, 2021, 374, 686-687. | 12.6 | 3 |
| 6 | Molecular reactions at aqueous interfaces. Nature Reviews Chemistry, 2020, 4, 459-475. | 30.2 | 149 |
| 7 | The Aqueous Surface as an Efficient Transient Stop for the Reactivity of Gaseous NO<sub>2</sub> in Liquid Water. Journal of the American Chemical Society, 2020, 142, 20937-20941. | 13.7 | 17 |
| 8 | Photoinduced Oxidation Reactions at the Airâ€“Water Interface. Journal of the American Chemical Society, 2020, 142, 16140-16155. | 13.7 | 38 |
| 9 | Isoprene Reactivity on Water Surfaces from abâ€…initio QM/MM Molecular Dynamics Simulations. ChemPhysChem, 2020, 21, 2263-2271. | 2.1 | 6 |
| 10 | Vibrational Sum-Frequency Generation Spectroscopy in the Energy Representation from Dual-Level Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2020, 124, 5675-5683. | 2.5 | 1 |
| 11 | Fast and Accurate Quantum Crystallography: From Small to Large, from Light to Heavy. Journal of Physical Chemistry Letters, 2019, 10, 6973-6982. | 4.6 | 48 |
| 12 | A New Mechanism of Acid Rain Generation from HOSO at the Airâ€“Water Interface. Journal of the American Chemical Society, 2019, 141, 16564-16568. | 13.7 | 39 |
| 13 | Photochemistry of HOSO radical in the gas phase. Journal of Chemical Physics, 2019, 151, 111103. | 3.0 | 13 |
| 14 | Theoretical Investigation of the Photoexcited NO<sub>2</sub>+H<sub>2</sub>O reaction at the Airâ€“Water Interface and Its Atmospheric Implications. Chemistry - A European Journal, 2019, 25, 13899-13904. | 3.3 | 14 |
| 15 | Vibrational Spectroscopy in Solution through Perturbative ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 4615-4622. | 5.3 | 9 |
| 16 | Molecular insights into the carbon dioxideâ€“carboxylate anion interactions and implications for carbon capture. Theoretical Chemistry Accounts, 2019, 138, 1. | 1.4 | 3 |
| 17 | Triplet state promoted reaction of SO<sub>2</sub> with H<sub>2</sub>O by competition between proton coupled electron transfer (pcet) and hydrogen atom transfer (hat) processes. Physical Chemistry Chemical Physics, 2019, 21, 9779-9784. | 2.8 | 27 |
| 18 | Transition-Metal-Free Approach for the Direct Arylation of Thiophene: Experimental and Theoretical Investigations towards the (Het)-Aryne Route. European Journal of Organic Chemistry, 2019, 2019, 547-556. | 2.4 | 9 |

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| 19 | Electronic Interactions in Iminophosphorane Superbase Complexes with Carbon Dioxide. Journal of Physical Chemistry A, 2018, 122, 1764-1770. | 2.5 | 3 |
| 20 | Photochemistry of SO<sub>2</sub> at the Airâ€“Water Interface: A Source of OH and HOSO Radicals. Journal of the American Chemical Society, 2018, 140, 12341-12344. | 13.7 | 42 |
| 21 | Cost-Effective Method for Free-Energy Minimization in Complex Systems with Elaborated Ab Initio Potentials. Journal of Chemical Theory and Computation, 2018, 14, 3262-3271. | 5.3 | 7 |
| 22 | Reaching multiâ€nanosecond timescales in combined QM/MM molecular dynamics simulations through parallel horsetail sampling. Journal of Computational Chemistry, 2017, 38, 659-668. | 3.3 | 19 |
| 23 | The atmospheric oxidation of CH<sub>3</sub>OOH by the OH radical: the effect of water vapor. Physical Chemistry Chemical Physics, 2017, 19, 12331-12342. | 2.8 | 28 |
| 24 | Highly accurate computation of free energies in complex systems through horsetail QM/MM molecular dynamics combined with free-energy perturbation theory. Theoretical Chemistry Accounts, 2017, 136, 1. | 1.4 | 9 |
| 25 | In vivo and in silico evaluation of a new nitric oxide donor, S,Sâ€² -dinitrosobucillamine. Nitric Oxide - Biology and Chemistry, 2017, 71, 32-43. | 2.7 | 3 |
| 26 | Physical Chemistry in France. ChemPhysChem, 2017, 18, 2558-2559. | 2.1 | 0 |
| 27 | Modeling Solvation in Supercritical CO<sub>2</sub>. ChemPhysChem, 2017, 18, 2560-2572. | 2.1 | 30 |
| 28 | Foreword to the special issue on the â€œElectronic Structure: Principles and Applications (ESPA 2016)â€• Conference. Theoretical Chemistry Accounts, 2017, 136, 1. | 1.4 | 0 |
| 29 | Impacts of cloud water droplets on the OH production rate from peroxide photolysis. Physical Chemistry Chemical Physics, 2017, 19, 31621-31627. | 2.8 | 11 |
| 30 | Computational Insights into the CH<sub>3</sub>Cl+OH Chemical Reaction Dynamics at the Airâ€“Water Interface. ChemPhysChem, 2017, 18, 2747-2755. | 2.1 | 4 |
| 31 | Geometry-dependent distributed polarizability models for the water molecule. Journal of Chemical Physics, 2016, 144, 034304. | 3.0 | 8 |
| 32 | The second Born approximation for the double ionization of N2by electron impact. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 135203. | 1.5 | 1 |
| 33 | Dipole and quadrupole polarizabilities of the water molecule as a function of geometry. Journal of Computational Chemistry, 2016, 37, 2125-2132. | 3.3 | 17 |
| 34 | Angular distributions in the double ionization of DNA bases by electron impact. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 225201. | 1.5 | 7 |
| 35 | Driving Forces Controlling Hostâ€“Guest Recognition in Supercritical Carbon Dioxide Solvent. Chemistry - A European Journal, 2016, 22, 2972-2979. | 3.3 | 10 |
| 36 | Structure and Stability Studies of Pharmacologically Relevant S-Nitrosothiols: A Theoretical Approach. Journal of Physical Chemistry A, 2016, 120, 4191-4200. | 2.5 | 18 |

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| 37 | Libraries of Extremely Localized Molecular Orbitals. 1. Model Molecules Approximation and Molecular Orbitals Transferability. Journal of Chemical Theory and Computation, 2016, 12, 1052-1067. | 5.3 | 64 |
| 38 | Structure of hydrogen tetroxide in gas phase and in aqueous environments: relationship to the hydroperoxyl radical self-reaction. Structural Chemistry, 2016, 27, 231-242. | 2.0 | 8 |
| 39 | Libraries of Extremely Localized Molecular Orbitals. 2. Comparison with the Pseudoatoms Transferability. Journal of Chemical Theory and Computation, 2016, 12, 1068-1081. | 5.3 | 48 |
| 40 | Preface to the ESPA-2014 special issue. Theoretical Chemistry Accounts, 2015, 134, 1. | 1.4 | 0 |
| 41 | Reactivity of aldehydes at the airâ€“water interface. Insights from molecular dynamics simulations and ab initio calculations. Organic and Biomolecular Chemistry, 2015, 13, 1673-1679. | 2.8 | 23 |
| 42 | Interconnection of Reactive Oxygen Species Chemistry across the Interfaces of Atmospheric, Environmental, and Biological Processes. Accounts of Chemical Research, 2015, 48, 575-583. | 15.6 | 90 |
| 43 | Solvation effects on electronic polarization and reactivity indices at the airâ€“water interface: insights from a theoretical study of cyanophenols. Theoretical Chemistry Accounts, 2015, 134, 1. | 1.4 | 13 |
| 44 | Unraveling the intramolecular cyclization mechanism of oxidized tryptophan in aqueous solution as a function of pH. Organic and Biomolecular Chemistry, 2015, 13, 8695-8702. | 2.8 | 4 |
| 45 | Hydration Effect on Amide I Infrared Bands in Water: An Interpretation Based on an Interaction Energy Decomposition Scheme. Journal of Physical Chemistry B, 2015, 119, 9056-9067. | 2.6 | 14 |
| 46 | Advances in QM/MM Molecular Dynamics Simulations of Chemical Processes at Aqueous Interfaces. Challenges and Advances in Computational Chemistry and Physics, 2015, , 303-324. | 0.6 | 5 |
| 47 | Evolution of the Coordinationâ€Sphere Symmetry in Copper(II), Nickel(II), and Zinc(II) Complexes with N,Nâ€²â€Doubleâ€Armed Diazaâ€Crown Ethers: Experimental and Theoretical Approaches. European Journal of Inorganic Chemistry, 2014, 2014, 4934-4945. | 2.0 | 9 |
| 48 | Theoretical insights on electron donorâ€“acceptor interactions involving carbon dioxide. Chemical Physics Letters, 2014, 601, 98-102. | 2.6 | 14 |
| 49 | Correlated ab initio molecular dynamics simulations of the acetoneâ€“carbon dioxide complex: implications for solubility in supercritical CO<sub>2</sub>. Molecular Simulation, 2014, 40, 154-159. | 2.0 | 8 |
| 50 | Toward Bis C,Câ€Glycosyl Compounds and Anomeric Îºâ€Glycoamino Acids through Michael Addition Reaction of Nitromethane on Z/E Pushâ€Pull Sugar Olefins. European Journal of Organic Chemistry, 2014, 2014, 7364-7376. | 2.4 | 9 |
| 51 | Water interactions with hydrophobic groups: Assessment and recalibration of semiempirical molecular orbital methods. Journal of Chemical Physics, 2014, 141, 034106. | 3.0 | 16 |
| 52 | Spectroscopic signatures of ozone at the airâ€“water interface and photochemistry implications. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11618-11623. | 7.1 | 58 |
| 53 | An ab initio analysis of the structure of l-tryptophan tautomers in microhydrated environments, in water and in hydrophobic solvents. Computational and Theoretical Chemistry, 2014, 1034, 17-25. | 2.5 | 5 |
| 54 | Vibrational Energy Relaxation of the Amide I Mode of N-Methylacetamide in D<sub>2</sub>O Studied through Bornâ€“Oppenheimer Molecular Dynamics. Journal of Physical Chemistry B, 2014, 118, 6186-6197. | 2.6 | 26 |

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| 55 | Preface to the ESPA-2012 special issue. Theoretical Chemistry Accounts, 2013, 132, 1. | 1.4 | 0 |
| 56 | A theoretical investigation of the CO2-philicity of amides and carbamides. Theoretical Chemistry Accounts, 2013, 132, 1. | 1.4 | 27 |
| 57 | Insights on peptide backbone Nâ€“H acidity: Structure of anions, hydration effects. Chemical Physics Letters, 2013, 561-562, 153-158. | 2.6 | 6 |
| 58 | Atmospheric Significance of Water Clusters and Ozoneâ€“Water Complexes. Journal of Physical Chemistry A, 2013, 117, 10381-10396. | 2.5 | 101 |
| 59 | Taste for Chiral Guests: Investigating the Stereoselective Binding of Peptides to Î²-Cyclodextrins. Journal of Physical Chemistry B, 2013, 117, 3091-3097. | 2.6 | 18 |
| 60 | Amino Acid Capture by Aqueous Interfaces. Implications for Biological Uptake. Journal of Physical Chemistry B, 2013, 117, 12469-12474. | 2.6 | 16 |
| 61 | Triple-differential cross sections for the ionization of thymine by electrons and positrons. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 175205. | 1.5 | 14 |
| 62 | Improvement of the Modeling of the Low-Temperature Oxidation of n-Butane: Study of the Primary Reactions. Journal of Physical Chemistry A, 2012, 116, 6142-6158. | 2.5 | 72 |
| 63 | Study of the Low Temperature Oxidation of Propane. Journal of Physical Chemistry A, 2012, 116, 12214-12228. | 2.5 | 57 |
| 64 | Intramolecular Interactions versus Hydration Effects on p-Guanidinoethyl-phenol Structure and pK<sub>a</sub> Values. Journal of Physical Chemistry A, 2012, 116, 9404-9411. | 2.5 | 14 |
| 65 | Is the HO<sub>4</sub><sup>â^’</sup> Anion a Key Species in the Aqueousâ€Phase Decomposition of Ozone?. Chemistry - A European Journal, 2012, 18, 13435-13445. | 3.3 | 11 |
| 66 | Reactivity of Volatile Organic Compounds at the Surface of a Water Droplet. Journal of the American Chemical Society, 2012, 134, 11821-11827. | 13.7 | 65 |
| 67 | Cavity Closure Dynamics of Peracetylated Î²-Cyclodextrins in Supercritical Carbon Dioxide. Journal of Physical Chemistry B, 2012, 116, 3982-3990. | 2.6 | 14 |
| 68 | Reactivity of Atmospherically Relevant Small Radicals at the Airâ€“Water Interface. Angewandte Chemie - International Edition, 2012, 51, 5413-5417. | 13.8 | 69 |
| 69 | Back Cover: Reactivity of Atmospherically Relevant Small Radicals at the Air-Water Interface (Angew.) Tj ETQq1 1 0.784314 rgBT /Ove | 13.8 | 1 |
| 70 | A New Glimpse into the CO<sub>2</sub>â€Philicity of Carbonyl Compounds. ChemPhysChem, 2012, 13, 3397-3403. | 2.1 | 44 |
| 71 | Peptide Binding to Î²-Cyclodextrins: Structure, Dynamics, Energetics, and Electronic Effects. Journal of Physical Chemistry A, 2011, 115, 11810-11817. | 2.5 | 19 |
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| 73 | Importance of Polarization and Charge Transfer Effects to Model the Infrared Spectra of Peptides in Solution. Journal of Chemical Theory and Computation, 2011, 7, 1840-1849. | 5.3 | 27 |
| 74 | Simulation of amino acid diffusion across water/hydrophobic interfaces. Physical Chemistry Chemical Physics, 2011, 13, 11579. | 2.8 | 14 |
| 75 | Reduction mechanism in class A methionine sulfoxide reductases: a theoretical chemistry investigation. Theoretical Chemistry Accounts, 2011, 129, 93-103. | 1.4 | 13 |
| 76 | Structure, stability, and dynamics of hydrogen polyoxides. International Journal of Quantum Chemistry, 2011, 111, 1543-1554. | 2.0 | 19 |
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| 78 | The gas phase reaction of carbonyl oxide with hydroxyl radical in presence of water vapor. A theoretical study on the reaction mechanism. Computational and Theoretical Chemistry, 2011, 965, 313-320. | 2.5 | 15 |
| 79 | An approach based on Density Functional Theory (DFT) calculations to assess the Candida antarctica lipase B selectivity in rutin, isoquercitrin and quercetin acetylation. Journal of Molecular Catalysis B: Enzymatic, 2010, 66, 325-331. | 1.8 | 21 |
| 80 | Glycine Dimers: Structure, Stability, and Medium Effects. ChemPhysChem, 2010, 11, 3499-3504. | 2.1 | 38 |
| 81 | Metalation of Pyridines with nBuLiâ€'Liâ€'Aminoalkoxide Mixed Aggregates: The Origin of Chemoselectivity. Journal of the American Chemical Society, 2010, 132, 2410-2416. | 13.7 | 38 |
| 82 | Theoretical Study of Chlorophyll a Hydrates Formation in Aqueous Organic Solvents. Journal of Physical Chemistry B, 2010, 114, 681-687. | 2.6 | 21 |
| 83 | Free energy calculations using dual-level Bornâ€“Oppenheimer molecular dynamics. Journal of Chemical Physics, 2010, 133, 064103. | 3.0 | 22 |
| 84 | Computer simulation of reactions in Î²-cyclodextrin molecular reactors: transition state recognition. Organic and Biomolecular Chemistry, 2010, 8, 4346. | 2.8 | 8 |
| 85 | Hyperconjugation in adjacent OO bonds: Remarkable odd/even effects. Chemical Physics Letters, 2009, 481, 180-182. | 2.6 | 20 |
| 86 | Six-coordination in Chlorophylls: The fundamental role of dispersion energy. Chemical Physics Letters, 2009, 472, 243-247. | 2.6 | 25 |
| 87 | Deamidation of Asparagine Residues: Direct Hydrolysis versus Succinimide-Mediated Deamidation Mechanisms. Journal of Physical Chemistry A, 2009, 113, 1111-1120. | 2.5 | 109 |
| 88 | Structure of Mixed Alkyllithium/Lithium Alkoxide Aggregates in Ethereal Solvents. Insights from Combined QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 6459-6467. | 2.6 | 14 |
| 89 | Theoretical Kinetic Study of the Reactions of Cycloalkylperoxy Radicals. Journal of Physical Chemistry A, 2009, 113, 6924-6935. | 2.5 | 51 |
| 90 | Combined ab initio and classical molecular dynamics simulations of alkyl-lithium aggregates in ethereal solutions. Theoretical Chemistry Accounts, 2008, 121, 321-326. | 1.4 | 8 |

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| 91 | Permeation selectivity of gaseous isotopes through dense polymers: Peculiar behavior of the hydrogen isotopes. Journal of Membrane Science, 2008, 318, 373-378. | 8.2 | 7 |
| 92 | Computational Study on Nonenzymatic Peptide Bond Cleavage at Asparagine and Aspartic Acid. Journal of Physical Chemistry A, 2008, 112, 8752-8761. | 2.5 | 57 |
| 93 | A Theoretical Study on nBuLi/Lithium Aminoalkoxide Aggregation in Hexane and THF. Journal of Organic Chemistry, 2008, 73, 9393-9402. | 3.2 | 33 |
| 94 | A theoretical study of medium effects on the structure of the glycine analogue aminomethylphosphonic acid. Physical Chemistry Chemical Physics, 2008, 10, 5624. | 2.8 | 9 |
| 95 | Theoretical Kinetic Study of Thermal Unimolecular Decomposition of Cyclic Alkyl Radicals. Journal of Physical Chemistry A, 2008, 112, 11598-11610. | 2.5 | 73 |
| 96 | The multipole moment expansion solvent continuum model: a brief review. Challenges and Advances in Computational Chemistry and Physics, 2008, , 23-38. | 0.6 | 10 |
| 97 | On the nature of the unusually long OO bond in HO3 and HO4 radicals. Physical Chemistry Chemical Physics, 2007, 9, 5865. | 2.8 | 51 |
| 98 | Theoretical Evaluation of the Substrate-Assisted Catalysis Mechanism for the Hydrolysis of Phosphate Monoester Dianions. Chemistry - A European Journal, 2007, 13, 3617-3629. | 3.3 | 31 |
| 99 | Theoretical study of solvent effects on the conformational equilibrium and electronic spectra of 2,2â€²-bipyridine derivatives. Computational and Theoretical Chemistry, 2007, 811, 169-174. | 1.5 | 16 |
| 100 | Extension of the composite CBS-QB3 method to singlet diradical calculations. Chemical Physics Letters, 2007, 435, 152-156. | 2.6 | 31 |
| 101 | Electron momentum spectroscopy of the valence orbitals of the water molecule in gas and liquid phase: A comparative study. Chemical Physics Letters, 2007, 439, 55-59. | 2.6 | 20 |
| 102 | Structure of levofloxacin in hydrophilic and hydrophobic media: Relationship to its antibacterial properties. Chemical Physics Letters, 2007, 442, 281-284. | 2.6 | 19 |
| 103 | Molecular dynamics of hydrogen peroxide in liquid water using a combined quantum/classical force field. Chemical Physics, 2007, 332, 341-347. | 1.9 | 73 |
| 104 | Can semi-empirical models describe HCl dissociation in water?. Theoretical Chemistry Accounts, 2007, 118, 425-435. | 1.4 | 23 |
| 105 | The structures of ozone and HOx radicals in aqueous solution from combined quantum/classical molecular dynamics simulations. Journal of Chemical Physics, 2006, 124, 194502. | 3.0 | 36 |
| 106 | Theoretical Study of the Reduction Mechanism of Sulfoxides by Thiols. Journal of Physical Chemistry A, 2006, 110, 7628-7636. | 2.5 | 33 |
| 107 | Detailed Kinetic Study of the Ring Opening of Cycloalkanes by CBS-QB3 Calculations. Journal of Physical Chemistry A, 2006, 110, 12693-12704. | 2.5 | 97 |
| 108 | Reaction Mechanism of Deamidation of Asparaginyl Residues in Peptides:Â Effect of Solvent Moleculesâ€. Journal of Physical Chemistry A, 2006, 110, 8354-8365. | 2.5 | 60 |

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| 109 | Analysis of interaction modes in calix[4]areneâ€“levofloxacin complexes by quantum methods. Journal of Physical Organic Chemistry, 2006, 19, 157-166. | 1.9 | 4 |
| 110 | The role of water on the acid-promoted E/Z isomerization of oximes in aqueous solution. Computational and Theoretical Chemistry, 2006, 764, 161-166. | 1.5 | 32 |
| 111 | Structure of the HOOO Radical in Liquid Water: A Theoretical Study. ChemPhysChem, 2006, 7, 463-467. | 2.1 | 24 |
| 112 | Comparison of three effective Hamiltonian models of increasing complexity: Triazene in water as a test case. Journal of Chemical Physics, 2006, 124, 214504. | 3.0 | 10 |
| 113 | Solvent effect on the radical addition reaction to double bond: Experimental and quantum chemical investigations. Chemical Physics Letters, 2005, 415, 202-205. | 2.6 | 21 |
| 114 | The Mechanism of Formamide Hydrolysis in Water from Ab Initio Calculations and Simulations. Chemistry - A European Journal, 2005, 11, 6743-6753. | 3.3 | 90 |
| 115 | Theoretical Study of the 1,3-Hydrogen Shift of Triazene in Water. Journal of Physical Chemistry B, 2005, 109, 23024-23030. | 2.6 | 16 |
| 116 | Dynamic and Electrostatic Effects in Enzymatic Processes. An Analysis of the Nucleophilic Substitution Reaction in Haloalkane Dehalogenase. Journal of the American Chemical Society, 2005, 127, 1946-1957. | 13.7 | 42 |
| 117 | Simulation of Liquid Water Using Semiempirical Hamiltonians and the Divide and Conquer Approach. Journal of Physical Chemistry A, 2005, 109, 3425-3432. | 2.5 | 60 |
| 118 | An improved semiempirical method for hydrated systems. Theoretical Chemistry Accounts, 2004, 112, 204. | 1.4 | 29 |
| 119 | Jean-Louis Rivail Honorary Issue. Theoretical Chemistry Accounts, 2004, 112, 179. | 1.4 | 0 |
| 120 | A Model for Double Asymmetric Induction in the Stereocontrolled Reduction of Glycosyl Î±-Ketoesters with Oxazaborolidines. Journal of the American Chemical Society, 2004, 126, 6996-7008. | 13.7 | 16 |
| 121 | Electrostatic component of solvation: Comparison of SCRF continuum models. Journal of Computational Chemistry, 2003, 24, 284-297. | 3.3 | 86 |
| 122 | Theoretical Study on the Alkaline and Neutral Hydrolysis of Succinimide Derivatives in Deamidation Reactions. Journal of Physical Chemistry A, 2002, 106, 11205-11214. | 2.5 | 27 |
| 123 | Rb+/Cs+selectivity of benzo and tribenzo derivatives of the 21C7 crown ether. A density functional study. Journal of Computational Chemistry, 2002, 23, 724-731. | 3.3 | 8 |
| 124 | An iterative procedure to determine Lennard-Jones parameters for their use in quantum mechanics/molecular mechanics liquid state simulations. Chemical Physics, 2002, 284, 607-614. | 1.9 | 21 |
| 125 | Theoretical study of photochemical processes involving singlet excited states of formaldehyde carbonyl oxide in the atmosphere. Chemical Physics, 2002, 285, 221-231. | 1.9 | 42 |
| 126 | Computer Simulation of Amide Bond Formation in Aqueous Solution. Journal of Physical Chemistry A, 2001, 105, 11574-11581. | 2.5 | 66 |

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| 127 | Theoretical study of hydrogenolysis termination processes in ethylene polymerization. Tetrahedron, 2001, 57, 2769-2774. | 1.9 | 12 |
| 128 | A QM/MM/continuum model for computations in solution: Comparison with QM/MM molecular dynamics simulations. International Journal of Quantum Chemistry, 2001, 84, 559-564. | 2.0 | 35 |
| 129 | A comparative study of two QM/MM methods testing the validity of the mean field approximation. Chemical Physics Letters, 2001, 344, 107-112. | 2.6 | 16 |
| 130 | Role of electronic polarization on the liquid phase affinity of calixareneâ€“crown-ethers towards alkali cations: a QM/MM molecular dynamics simulation. Chemical Physics, 2001, 272, 47-59. | 1.9 | 12 |
| 131 | Molecular dynamics simulation of carbonyl oxide in acetonitrile using combined DFT/MM potentials. Computational and Theoretical Chemistry, 2001, 536, 1-7. | 1.5 | 3 |
| 132 | Theoretical study of selectivity mechanisms in propylene polymerization with metallocene catalysts. Computational and Theoretical Chemistry, 2001, 541, 227-235. | 1.5 | 18 |
| 133 | The reaction field of a water molecule in liquid water: Comparison of different quantum/classical models. Journal of Chemical Physics, 2001, 115, 5220-5227. | 3.0 | 35 |
| 134 | Improving description of hydrogen bonds at the semiempirical level: water-water interactions as test case. Journal of Computational Chemistry, 2000, 21, 572-581. | 3.3 | 70 |
| 135 | New approaches to the description of short-range repulsion interactions in hybrid quantum/classical systems. Chemical Physics Letters, 2000, 329, 154-159. | 2.6 | 20 |
| 136 | On the tautomerization process of glycine in aqueous solution. Chemical Physics Letters, 2000, 321, 433-437. | 2.6 | 57 |
| 137 | Basic ideas for the correction of semiempirical methods describing H-bonded systems. Chemical Physics Letters, 2000, 330, 118-124. | 2.6 | 66 |
| 138 | Intramolecular proton transfer of serine in aqueous solution. Mechanism and energetics. Theoretical Chemistry Accounts, 2000, 104, 89-95. | 1.4 | 34 |
| 139 | Insights in the Peptide Hydrolysis Mechanism by Thermolysin: A Theoretical QM/MM study. Journal of Molecular Modeling, 2000, 6, 527-538. | 1.8 | 86 |
| 140 | Theoretical Investigation of Reaction Mechanisms for Carboxylic Acid Formation in the Atmosphere. Journal of the American Chemical Society, 2000, 122, 8990-8997. | 13.7 | 79 |
| 141 | Theoretical Study of Formic Acid Anhydride Formation from Carbonyl Oxide in the Atmosphere. Journal of Physical Chemistry A, 2000, 104, 380-388. | 2.5 | 53 |
| 142 | Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. Journal of Physical Chemistry A, 2000, 104, 10923-10931. | 2.5 | 54 |
| 143 | Effect of solvent fluctuations on proton transfer dynamics: a hybrid AM1/MM molecular dynamics simulation on the [H3Nâ€“Hâ€“NH3]+ system. Chemical Physics, 1999, 240, 93-99. | 1.9 | 9 |
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| 145 | Modeling ?-lactam interactions in aqueous solution through combined quantum mechanics-molecular mechanics methods. Journal of Computational Chemistry, 1999, 20, 1401-1411. | 3.3 | 16 |
| 146 | A Density Functional Study on the Coordination of Aldehydes to N-Sulfonyl 1,3,2-Oxazaborolidin-5-one. Journal of the American Chemical Society, 1999, 121, 10772-10780. | 13.7 | 15 |
| 147 | Molecular dynamics simulation of formamide in water using density functional theory and classical potentials. Journal of Chemical Physics, 1999, 111, 1117-1125. | 3.0 | 41 |
| 148 | Theoretical Study of the Mechanisms of Ethylene Polymerization with Metallocene-Type Catalysts. Journal of Physical Chemistry B, 1999, 103, 27-35. | 2.6 | 26 |
| 149 | Combined AM1/MM3 computations on organic systems: the Dielsâ€“Alder reaction as a test case. Chemical Physics Letters, 1998, 296, 239-244. | 2.6 | 7 |
| 150 | AM1/TIP3P molecular dynamics simulation of imidazole proton-relay processes in aqueous solution. Chemical Physics Letters, 1998, 297, 38-44. | 2.6 | 10 |
| 151 | Ab initio calculations of tautomer equilibrium and protonation enthalpy of 4- and 5-methylimidazole in the gas phase: Basis set and correlation effects. Computational and Theoretical Chemistry, 1998, 422, 197-204. | 1.5 | 37 |
| 152 | Density functional studies of compounds involved in atmospheric chemistry: nitrogen oxides. Computational and Theoretical Chemistry, 1998, 426, 95-104. | 1.5 | 12 |
| 153 | Theoretical Study of the [2+2] Cycloaddition of Thioketenes with Imines To FormÎ²-Thiolactams. Chemistry - A European Journal, 1998, 4, 328-334. | 3.3 | 9 |
| 154 | Influence of environment on proton-transfer mechanisms in model triads from theoretical calculations. Journal of Computational Chemistry, 1998, 19, 1675-1688. | 3.3 | 27 |
| 155 | Theoretical study of ester enolate-imine condensation route to ?-lactams. Journal of Computational Chemistry, 1998, 19, 1826-1833. | 3.3 | 9 |
| 156 | The Role of Menthyl Group in Catalyzed Asymmetric Dielsâ^'Alder Reactions. A Combined Quantum Mechanics/Molecular Mechanics Study. Journal of Organic Chemistry, 1998, 63, 4664-4670. | 3.2 | 15 |
| 157 | Self-Consistent Reaction Field Calculations of Nonequilibrium Solvent Effects on Proton Transfer Processes through Low-Barrier Hydrogen Bonds. Journal of Physical Chemistry A, 1998, 102, 10728-10735. | 2.5 | 15 |
| 158 | Neutral and Alkaline Hydrolyses of Model Î²-Lactam Antibiotics. An ab Initio Study of Water Catalysis. Journal of the American Chemical Society, 1998, 120, 2146-2155. | 13.7 | 71 |
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