# Miquel Huix-Rotllant

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 35 papers | 1,536 citations | 17 h-index | 39 g-index |
| 44 ext. papers | 1,735 ext. citations | 5.4 avg, IF | 5.17 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 35 | Impact of the Dynamic Electron Correlation on the Unusually Long Excited-State Lifetime of Thymine. *Journal of Physical Chemistry Letters*, **2021**, 12, 4339-4346 | 6.4 | 9 |
| 34 | Analytic Energy, Gradient, and Hessian of Electrostatic Embedding QM/MM Based on Electrostatic Potential-Fitted Atomic Charges Scaling Linearly with the MM Subsystem Size. *Journal of Chemical Theory and Computation*, **2021**, 17, 538-548 | 6.4 | 5 |
| 33 | Infrared spectroscopy from electrostatic embedding QM/MM: local normal mode analysis of infrared spectra of arabidopsis thaliana plant cryptochrome. *Physical Chemistry Chemical Physics*, **2021**, 23, 1666-1674 | 3.6 | 2 |
| 32 | Ultrafast Intersystem Crossing in Xanthone from Wavepacket Dynamics.. *Journal of the American Chemical Society*, **2021**, 143, 21474-21477 | 16.4 | 2 |
| 31 | UV-visible absorption spectrum of FAD and its reduced forms embedded in a cryptochrome protein. *Physical Chemistry Chemical Physics*, **2020**, 22, 12447-12455 | 3.6 | 17 |
| 30 | Efficient Analytic Second Derivative of Electrostatic Embedding QM/MM Energy: Normal Mode Analysis of Plant Cryptochrome. *Journal of Chemical Theory and Computation*, **2020**, 16, 3816-3824 | 6.4 | 12 |
| 29 | Time-Dependent Density Functional Theory **2020**, 13-46 | | 6 |
| 28 | Impact of the redox state of flavin chromophores on the UV□is spectra, redox and acidity constants and electron affinities. *Journal of Photochemistry and Photobiology A: Chemistry*, **2020**, 387, 112164 | 4.7 | 10 |
| 27 | Theoretical insights into the formation and stability of radical oxygen species in cryptochromes. *Physical Chemistry Chemical Physics*, **2019**, 21, 8874-8882 | 3.6 | 12 |
| 26 | Analytic QM/MM atomic charge derivatives avoiding the scaling of coupled perturbed equations with the MM subsystem size. *Journal of Chemical Physics*, **2019**, 151, 041102 | 3.9 | 7 |
| 25 | Ultrafast photochemistry of free-base porphyrin: a theoretical investigation of B -vQ internal conversion mediated by dark states. *Physical Chemistry Chemical Physics*, **2018**, 20, 12483-12492 | 3.6 | 6 |
| 24 | Ultrafast carbon monoxide photolysis and heme spin-crossover in myoglobin via nonadiabatic quantum dynamics. *Nature Communications*, **2018**, 9, 4502 | 17.4 | 34 |
| 23 | Sampling the protonation states: the pH-dependent UV absorption spectrum of a polypeptide dyad. *Physical Chemistry Chemical Physics*, **2018**, 20, 23252-23261 | 3.6 | 10 |
| 22 | Description of Conical Intersections with Density Functional Methods. *Topics in Current Chemistry*, **2016**, 368, 445-76 | | 27 |
| 21 | High-Energy Long-Lived Mixed Frenkel-Charge-Transfer Excitons: From Double Stranded (AT)n to Natural DNA. *Chemistry - A European Journal*, **2016**, 22, 4904-14 | 4.8 | 16 |
| 20 | Many-Body Perturbation Theory (MBPT) and Time-Dependent Density-Functional Theory (TD-DFT): MBPT Insights About What Is Missing In, and Corrections To, the TD-DFT Adiabatic Approximation. *Topics in Current Chemistry*, **2016**, 368, 1-60 | | 17 |
| 19 | Population of triplet states in acetophenone: A quantum dynamics perspective. *Comptes Rendus Chimie*, **2016**, 19, 50-56 | 2.7 | 10 |

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| 18 | An Effective Procedure for Analyzing Molecular Vibrations in Terms of Local Fragment Modes. *Journal of Chemical Theory and Computation*, **2016**, 12, 4768-4777 | 6.4 | 10 |
| 17 | Concurrent Effects of Delocalization and Internal Conversion Tune Charge Separation at Regioregular Polythiophene-Fullerene Heterojunctions. *Journal of Physical Chemistry Letters*, **2015**, 6, 1702-8 | 6.4 | 67 |
| 16 | Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations. *Journal of Chemical Physics*, **2015**, 142, 184104 | 3.9 | 31 |
| 15 | First-Principles Quantum Dynamics of Singlet Fission: Coherent versus Thermally Activated Mechanisms Governed by Molecular π Stacking. *Physical Review Letters*, **2015**, 115, 107401 | 7.4 | 122 |
| 14 | Stabilization of Mixed Frenkel-Charge Transfer Excitons Extended Across Both Strands of Guanine-Cytosine DNA Duplexes. *Journal of Physical Chemistry Letters*, **2015**, 6, 2247-51 | 6.4 | 27 |
| 13 | Photophysics of acetophenone interacting with DNA: why the road to photosensitization is open. *Photochemistry and Photobiology*, **2015**, 91, 323-30 | 3.6 | 14 |
| 12 | Assessment of approximate computational methods for conical intersections and branching plane vectors in organic molecules. *Journal of Chemical Physics*, **2014**, 141, 124122 | 3.9 | 56 |
| 11 | Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. *Journal of Chemical Theory and Computation*, **2014**, 10, 3074-84 | 6.4 | 132 |
| 10 | Theoretical study of the photochemical initiation in nitroxide-mediated photopolymerization. *Journal of Physical Chemistry A*, **2014**, 118, 4464-70 | 2.8 | 11 |
| 9 | Assessment of density functional theory based SCF (self-consistent field) and linear response methods for longest wavelength excited states of extended π conjugated molecular systems. *Journal of Chemical Physics*, **2014**, 141, 024112 | 3.9 | 35 |
| 8 | Triplet state photochemistry and the three-state crossing of acetophenone within time-dependent density-functional theory. *Journal of Chemical Physics*, **2014**, 140, 134305 | 3.9 | 14 |
| 7 | Assessment of Density Functional Theory for Describing the Correlation Effects on the Ground and Excited State Potential Energy Surfaces of a Retinal Chromophore Model. *Journal of Chemical Theory and Computation*, **2013**, 9, 3917-32 | 6.4 | 78 |
| 6 | Theoretical study of the photochemical generation of triplet acetophenone. *Physical Chemistry Chemical Physics*, **2013**, 15, 19293-300 | 3.6 | 25 |
| 5 | Progress in time-dependent density-functional theory. *Annual Review of Physical Chemistry*, **2012**, 63, 287-323 | 15.7 | 543 |
| 4 | Assessment of dressed time-dependent density-functional theory for the low-lying valence states of 28 organic chromophores. *Chemical Physics*, **2011**, 391, 120-129 | 2.3 | 66 |
| 3 | Assessment of noncollinear spin-flip Tamm-Dancoff approximation time-dependent density-functional theory for the photochemical ring-opening of oxirane. *Physical Chemistry Chemical Physics*, **2010**, 12, 12811-25 | 3.6 | 81 |
| 2 | Characterization of optical spectra of interacting systems: Application to oxide-supported metal clusters. *International Journal of Quantum Chemistry*, **2008**, 108, 2978-2990 | 2.1 | 3 |
| 1 | Simulation of photoelectron spectra with anharmonicity fully included: Application to the X 2A2. *Journal of Chemical Physics*, **2006**, 125, 014311 | 3.9 | 17 |