

Miquel Huix-Rotllant

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Progress in time-dependent density-functional theory. <i>Annual Review of Physical Chemistry</i> , 2012 , 63, 287-323	15.7	543
34	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3074-84	6.4	132
33	First-Principles Quantum Dynamics of Singlet Fission: Coherent versus Thermally Activated Mechanisms Governed by Molecular π -Stacking. <i>Physical Review Letters</i> , 2015 , 115, 107401	7.4	122
32	Assessment of noncollinear spin-flip Tamm-Dancoff approximation time-dependent density-functional theory for the photochemical ring-opening of oxirane. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 12811-25	3.6	81
31	Assessment of Density Functional Theory for Describing the Correlation Effects on the Ground and Excited State Potential Energy Surfaces of a Retinal Chromophore Model. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3917-32	6.4	78
30	Concurrent Effects of Delocalization and Internal Conversion Tune Charge Separation at Regioregular Polythiophene-Fullerene Heterojunctions. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 1702-8	6.4	67
29	Assessment of dressed time-dependent density-functional theory for the low-lying valence states of 28 organic chromophores. <i>Chemical Physics</i> , 2011 , 391, 120-129	2.3	66
28	Assessment of approximate computational methods for conical intersections and branching plane vectors in organic molecules. <i>Journal of Chemical Physics</i> , 2014 , 141, 124122	3.9	56
27	Assessment of density functional theory based BCF (self-consistent field) and linear response methods for longest wavelength excited states of extended π -conjugated molecular systems. <i>Journal of Chemical Physics</i> , 2014 , 141, 024112	3.9	35
26	Ultrafast carbon monoxide photolysis and heme spin-crossover in myoglobin via nonadiabatic quantum dynamics. <i>Nature Communications</i> , 2018 , 9, 4502	17.4	34
25	Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations. <i>Journal of Chemical Physics</i> , 2015 , 142, 184104	3.9	31
24	Description of Conical Intersections with Density Functional Methods. <i>Topics in Current Chemistry</i> , 2016 , 368, 445-76		27
23	Stabilization of Mixed Frenkel-Charge Transfer Excitons Extended Across Both Strands of Guanine-Cytosine DNA Duplexes. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 2247-51	6.4	27
22	Theoretical study of the photochemical generation of triplet acetophenone. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 19293-300	3.6	25
21	UV-visible absorption spectrum of FAD and its reduced forms embedded in a cryptochrome protein. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 12447-12455	3.6	17
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. <i>Topics in Current Chemistry</i> , 2016 , 368, 1-60		17
19	Simulation of photoelectron spectra with anharmonicity fully included: Application to the X 2A ₂ . <i>Journal of Chemical Physics</i> , 2006 , 125, 014311	3.9	17

18	High-Energy Long-Lived Mixed Frenkel-Charge-Transfer Excitons: From Double Stranded (AT) _n to Natural DNA. <i>Chemistry - A European Journal</i> , 2016 , 22, 4904-14	4.8	16
17	Photophysics of acetophenone interacting with DNA: why the road to photosensitization is open. <i>Photochemistry and Photobiology</i> , 2015 , 91, 323-30	3.6	14
16	Triplet state photochemistry and the three-state crossing of acetophenone within time-dependent density-functional theory. <i>Journal of Chemical Physics</i> , 2014 , 140, 134305	3.9	14
15	Theoretical insights into the formation and stability of radical oxygen species in cryptochromes. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 8874-8882	3.6	12
14	Efficient Analytic Second Derivative of Electrostatic Embedding QM/MM Energy: Normal Mode Analysis of Plant Cryptochrome. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3816-3824	6.4	12
13	Theoretical study of the photochemical initiation in nitroxide-mediated photopolymerization. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 4464-70	2.8	11
12	Population of triplet states in acetophenone: A quantum dynamics perspective. <i>Comptes Rendus Chimie</i> , 2016 , 19, 50-56	2.7	10
11	An Effective Procedure for Analyzing Molecular Vibrations in Terms of Local Fragment Modes. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4768-4777	6.4	10
10	Impact of the redox state of flavin chromophores on the UV-vis spectra, redox and acidity constants and electron affinities. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020 , 387, 112164	4.7	10
9	Sampling the protonation states: the pH-dependent UV absorption spectrum of a polypeptide dyad. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 23252-23261	3.6	10
8	Impact of the Dynamic Electron Correlation on the Unusually Long Excited-State Lifetime of Thymine. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4339-4346	6.4	9
7	Analytic QM/MM atomic charge derivatives avoiding the scaling of coupled perturbed equations with the MM subsystem size. <i>Journal of Chemical Physics</i> , 2019 , 151, 041102	3.9	7
6	Ultrafast photochemistry of free-base porphyrin: a theoretical investigation of B ₁₀ internal conversion mediated by dark states. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 12483-12492	3.6	6
5	Time-Dependent Density Functional Theory 2020 , 13-46		6
4	Analytic Energy, Gradient, and Hessian of Electrostatic Embedding QM/MM Based on Electrostatic Potential-Fitted Atomic Charges Scaling Linearly with the MM Subsystem Size. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 538-548	6.4	5
3	Characterization of optical spectra of interacting systems: Application to oxide-supported metal clusters. <i>International Journal of Quantum Chemistry</i> , 2008 , 108, 2978-2990	2.1	3
2	Infrared spectroscopy from electrostatic embedding QM/MM: local normal mode analysis of infrared spectra of arabidopsis thaliana plant cryptochrome. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 1666-1674	3.6	2
1	Ultrafast Intersystem Crossing in Xanthone from Wavepacket Dynamics.. <i>Journal of the American Chemical Society</i> , 2021 , 143, 21474-21477	16.4	2

