Carles Curutchet

List of Publications by Year
in descending order

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78 papers	4,117 citations	94269 37 h-index	114278 63 g-index
79 all docs	79 docs citations	79 times ranked	3739 citing authors

#	Article	IF	Citations
1	Beyond FÃ¶rster Resonance Energy Transfer in Biological and Nanoscale Systems. Journal of Physical Chemistry B, 2009, 113, 6583-6599.	1.2	404
2	Quantum Chemical Studies of Light Harvesting. Chemical Reviews, 2017, 117, 294-343.	23.0	262
3	Electronic Energy Transfer in Condensed Phase Studied by a Polarizable QM/MM Model. Journal of Chemical Theory and Computation, 2009, 5, 1838-1848.	2.3	259
4	On the Performance of Continuum Solvation Methods. A Comment on â€œUniversal Approaches to Solvation Modelingâ€• Accounts of Chemical Research, 2009, 42, 489-492.	7.6	171
5	How Solvent Controls Electronic Energy Transfer and Light Harvesting. Journal of Physical Chemistry B, 2007, 111, 6978-6982.	1.2	167
6	Photosynthetic Light-Harvesting Is Tuned by the Heterogeneous Polarizable Environment of the Protein. Journal of the American Chemical Society, 2011, 133, 3078-3084.	6.6	123
7	Solvation in octanol: parametrization of the continuum MST model. Journal of Computational Chemistry, 2001, 22, 1180-1193.	1.5	120
8	Fretting about FRET: Failure of the Ideal Dipole Approximation. Biophysical Journal, 2009, 96, 4779-4788.	0.2	118
9	How Solvent Controls Electronic Energy Transfer and Light Harvesting:â€‰ Toward a Quantum-Mechanical Description of Reaction Field and Screening Effects. Journal of Physical Chemistry B, 2007, 111, 13253-13265.	1.2	117
10	Examining FÃ¶rster Energy Transfer for Semiconductor Nanocrystalline Quantum Dot Donors and Acceptors. Journal of Physical Chemistry C, 2008, 112, 13336-13341.	1.5	104
11	Resonance energy transfer: Beyond the limits. Laser and Photonics Reviews, 2011, 5, 114-123.	4.4	93
12	Continuum solvation models: Dissecting the free energy of solvation. Physical Chemistry Chemical Physics, 2003, 5, 3827-3836.	1.3	89
13	Electrostatic component of solvation: Comparison of SCRF continuum models. Journal of Computational Chemistry, 2003, 24, 284-297.	1.5	86
14	Toward a Molecular Scale Interpretation of Excitation Energy Transfer in Solvated Bichromophoric Systems. Journal of the American Chemical Society, 2005, 127, 16733-16744.	6.6	85
15	Extension of the MST model to the IEF formalism: HF and B3LYP parametrizations. Computational and Theoretical Chemistry, 2005, 727, 29-40.	1.5	79
16	A Subsystem TDDFT Approach for Solvent Screening Effects on Excitation Energy Transfer Couplings. Journal of Chemical Theory and Computation, 2010, 6, 1843-1851.	2.3	77
17	Toward a Unified Modeling of Environment and Bridge-Mediated Contributions to Electronic Energy Transfer: A Fully Polarizable QM/MM/PCM Approach. Journal of Chemical Theory and Computation, 2012, 8, 4462-4473.	2.3	69
18	Excitation Dynamics in Phycoerythrin 545: Modeling of Steady-State Spectra and Transient Absorption with Modified Redfield Theory. Biophysical Journal, 2010, 99, 344-352.	0.2	67

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19	Does FÃ¶rster Theory Predict the Rate of Electronic Energy Transfer for a Model Dyad at Low Temperature?. Journal of Physical Chemistry B, 2008, 112, 3759-3766.	1.2	65
20	The Fennaâ€“Matthewsâ€“Olson Protein Revisited: A Fully Polarizable (TD)DFT/MM Description. ChemPhysChem, 2014, 15, 3194-3204.	1.0	65
21	Chromophoreâ€“Protein Coupling beyond Nonpolarizable Models: Understanding Absorption in Green Fluorescent Protein. Journal of Chemical Theory and Computation, 2015, 11, 4825-4839.	2.3	65
22	Ultrafast light harvesting dynamics in the cryptophyte phycocyanin 645. Photochemical and Photobiological Sciences, 2007, 6, 964-975.	1.6	62
23	Ideal dipole approximation fails to predict electronic coupling and energy transfer between semiconducting single-wall carbon nanotubes. Journal of Chemical Physics, 2009, 130, 081104.	1.2	56
24	Towards a Molecular Scale Interpretation of Excitation Energy Transfer in Solvated Bichromophoric Systems. II. The Through-Bond Contribution. Journal of Physical Chemistry B, 2007, 111, 853-863.	1.2	55
25	Quantum mechanical methods applied to excitation energy transfer: A comparative analysis on excitation energies and electronic couplings. Journal of Chemical Physics, 2008, 129, 034104.	1.2	54
26	Shared-mode assisted resonant energy transfer in the weak coupling regime. Journal of Chemical Physics, 2009, 130, 214505.	1.2	53
27	The role of the environment in electronic energy transfer: a molecular modeling perspective. Physical Chemistry Chemical Physics, 2011, 13, 11538.	1.3	53
28	Toward Reliable Prediction of the Energy Ladder in Multichromophoric Systems: A Benchmark Study on the FMO Light-Harvesting Complex. Journal of Chemical Theory and Computation, 2013, 9, 4928-4938.	2.3	52
29	Geometry Optimization in Polarizable QM/MM Models: The Induced Dipole Formulation. Journal of Chemical Theory and Computation, 2014, 10, 1588-1598.	2.3	52
30	Theoretical Characterization of the Spectral Density of the Water-Soluble Chlorophyll-Binding Protein from Combined Quantum Mechanics/Molecular Mechanics Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 5826-5837.	2.3	51
31	Dispersion and repulsion contributions to the solvation free energy: Comparison of quantum mechanical and classical approaches in the polarizable continuum model. Journal of Computational Chemistry, 2006, 27, 1769-1780.	1.5	49
32	Energy Flow in the Cryptophyte PE545 Antenna Is Directed by Bilin Pigment Conformation. Journal of Physical Chemistry B, 2013, 117, 4263-4273.	1.2	49
33	Analysis of the Effects ofN-Substituents on Some Aspects of the Aromaticity of Imidazoles and Pyrazoles. Journal of Physical Chemistry A, 2011, 115, 8571-8577.	1.1	46
34	MST Continuum Study of the Hydration Free Energies of Monovalent Ionic Species. Journal of Physical Chemistry B, 2005, 109, 3565-3574.	1.2	44
35	Molecular basis of the excitonâ€“phonon interactions in the PE545 light-harvesting complex. Physical Chemistry Chemical Physics, 2014, 16, 16302-16311.	1.3	43
36	Polarizable QM/MM Multiconfiguration Self-Consistent Field Approach with State-Specific Corrections: Environment Effects on Cytosine Absorption Spectrum. Journal of Chemical Theory and Computation, 2015, 11, 1674-1682.	2.3	43

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37	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913.	2.3	41
38	On the Binding of Congo Red to Amyloid Fibrils. Angewandte Chemie - International Edition, 2020, 59, 8104-8107.	7.2	36
39	Limits and potentials of quantum chemical methods in modelling photosynthetic antennae. Physical Chemistry Chemical Physics, 2015, 17, 30783-30792.	1.3	34
40	Superexchange-mediated electronic energy transfer in a model dyad. Physical Chemistry Chemical Physics, 2010, 12, 7378.	1.3	32
41	Electronic energy transfer in biomacromolecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1392.	6.2	30
42	Measurement of Electronâ^'Electron Interactions and Correlations Using Two-Dimensional Electronic Double-Quantum Coherence Spectroscopy. Journal of Physical Chemistry A, 2009, 113, 12122-12133.	1.1	28
43	Tripletâ€“Triplet Energy Transfer in DNA: A Process that Occurs on the Nanosecond Timescale. Angewandte Chemie - International Edition, 2011, 50, 1820-1822.	7.2	28
44	Synthesis, characterization and DFT calculations of new ethynyl-bridged C60 derivatives. Tetrahedron, 2010, 66, 4230-4242.	1.0	26
45	Impact of Electronic Fluctuations and Their Description on the Exciton Dynamics in the Light-Harvesting Complex PE545. Journal of Physical Chemistry B, 2017, 121, 1330-1339.	1.2	26
46	Delocalization-Enhanced Long-Range Energy Transfer between Cryptophyte Algae PE545 Antenna Proteins. Journal of Physical Chemistry B, 2011, 115, 5243-5253.	1.2	25
47	Electrostatic versus Resonance Interactions in Photoreceptor Proteins: The Case of Rhodopsin. Journal of Physical Chemistry Letters, 2016, 7, 4547-4553.	2.1	25
48	Distance Dependence of Triplet Energy Transfer in Water and Organic Solvents: A QM/MD Study. Journal of Physical Chemistry C, 2012, 116, 22179-22185.	1.5	24
49	Spatial and Electronic Correlations in the PE545 Light-Harvesting Complex. Journal of Physical Chemistry Letters, 2013, 4, 372-377.	2.1	24
50	Density-Dependent Formulation of Dispersionâ€“Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. Journal of Chemical Theory and Computation, 2018, 14, 1671-1681.	2.3	24
51	Binding of 13-Amidohuprines to Acetylcholinesterase:Â Exploring the Ligand-Induced Conformational Change of the Gly117-Gly118 Peptide Bond in the Oxyanion Hole. Journal of Medicinal Chemistry, 2006, 49, 6833-6840.	2.9	19
52	Structural and energetic study of cationâ€“Ïâ€“cation interactions in proteins. Physical Chemistry Chemical Physics, 2017, 19, 9849-9861.	1.3	19
53	Prediction of pH-Dependent Hydrophobic Profiles of Small Molecules from Miertusâ€“Scroccoâ€“Tomasi Continuum Solvation Calculations. Journal of Physical Chemistry B, 2017, 121, 9868-9880.	1.2	16
54	Transferability and additivity of dihedral parameters in polarizable and nonpolarizable empirical force fields. Journal of Computational Chemistry, 2015, 36, 1874-1884.	1.5	15

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55	Spectral Variability in Phycocyanin Cryptophyte Antenna Complexes is Controlled by Changes in the Î±â€Polypeptide Chains. ChemPhotoChem, 2019, 3, 945-956.	1.5	15
56	Energy decomposition in molecular complexes: Implications for the treatment of polarization in molecular simulations. Journal of Computational Chemistry, 2003, 24, 1263-1275.	1.5	14
57	Self-consistent quantum mechanical model for the description of excitation energy transfers in molecules at interfaces. Journal of Chemical Physics, 2006, 125, 054710.	1.2	14
58	The DNA-forming properties of 6-selenoguanine. Physical Chemistry Chemical Physics, 2014, 16, 1101-1110.	1.3	13
59	Electronic Energy Transfer in Photosynthetic Antenna Systems. Springer Series in Chemical Physics, 2009, , 3-34.	0.2	13
60	Electronic Couplings for Resonance Energy Transfer from CCSD Calculations: From Isolated to Solvated Systems. Journal of Chemical Theory and Computation, 2015, 11, 5219-5228.	2.3	12
61	Transferability of fragmental contributions to the octanol/water partition coefficient: An NDDO-based MST study. Journal of Computational Chemistry, 2003, 24, 32-45.	1.5	11
62	Determination of the protonation preferences of bilin pigments in cryptophyte antenna complexes. Physical Chemistry Chemical Physics, 2018, 20, 21404-21416.	1.3	11
63	Prediction of the n-octanol/water partition coefficients in the SAMPL6 blind challenge from MST continuum solvation calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 443-451.	1.3	11
64	On the Binding of Congo Red to Amyloid Fibrils. Angewandte Chemie, 2020, 132, 8181-8184.	1.6	11
65	Can FÃ¶rster Theory Describe Stereoselective Energy Transfer Dynamics in a Proteinâ€“Ligand Complex?. Journal of Physical Chemistry B, 2017, 121, 2265-2278.	1.2	10
66	Prediction of n-octanol/water partition coefficients and acidity constants (pKa) in the SAMPL7 blind challenge with the IEFPCM-MST model. Journal of Computer-Aided Molecular Design, 2021, 35, 803-811.	1.3	10
67	Environment effects on tripletâ€“triplet energy transfer in DNA. Chemical Physics Letters, 2011, 512, 118-122.	1.2	7
68	MST study of group contributions for alkane derivatives: effect of the charge normalization. Chemical Physics Letters, 2004, 384, 299-305.	1.2	6
69	Quantum mechanical study of the solvent-dependence of electronic energy transfer rates in a Bodipy closely-spaced dyad. Photochemical and Photobiological Sciences, 2011, 10, 1602-1609.	1.6	6
70	Dissecting the Nature of Exciton Interactions in Ethyne-Linked Tetraarylporphyrin Arrays. Journal of Physical Chemistry C, 2013, 117, 12423-12431.	1.5	6
71	How abasic sites impact hole transfer dynamics in GC-rich DNA sequences. Physical Chemistry Chemical Physics, 2018, 20, 23123-23131.	1.3	6
72	Prediction of Conformational Free Energy Differences of Solutes in Solutionâ¶ An MC-MST Study. Molecular Simulation, 2002, 28, 153-171.	0.9	5

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73	Single Amino Acid Mutation Controls Hole Transfer Dynamics in DNA-Methyltransferase Hha I Complexes. Journal of Physical Chemistry Letters, 2015, 6, 3749-3753.	2.1	5
74	Solute-Solvent Interactions from QM SCRF Methods. , 2004, , 475-495.		2
75	How the Molecular Environment Controls Excitation Energy Transfer and Light Harvesting: a Quantum Mechanical Model. AIP Conference Proceedings, 2007, , .	0.3	1
76	Fretting About FRET: Breakdown of the Ideal Dipole Approximation. Biophysical Journal, 2010, 98, 582a.	0.2	1
77	Quantum-Coherent Energy Transfer in Marine Algae at Ambient Temperature via Ultrafast Photon Echo Studies. , 2010, , .		1
78	Through-bond Versus Through-Space Contributions on Excitation Energy Transfer in Condensed Phase. AIP Conference Proceedings, 2007, , .	0.3	0