Benedetta Mennucci

List of Publications by Year
in descending order

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330	51,260	8181	1424
papers	citations	76 h-index	221 g-index

343	343	343	32320
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum Mechanical Continuum Solvation Models. Chemical Reviews, 2005, 105, 2999-3094.	47.7	14,149
2	A new integral equation formalism for the polarizable continuum model: Theoretical background and applications to isotropic and anisotropic dielectrics. Journal of Chemical Physics, 1997, 107, 3032-3041.	3.0	5,950
3	Continuum solvation models: A new approach to the problem of soluteâ€™s charge distribution and cavity boundaries. Journal of Chemical Physics, 1997, 106, 5151-5158.	3.0	2,463
4	The IEF version of the PCM solvation method: an overview of a new method addressed to study molecular solutes at the QM ab initio level. Computational and Theoretical Chemistry, 1999, 464, 211-226.	1.5	2,157
5	Evaluation of Solvent Effects in Isotropic and Anisotropic Dielectrics and in Ionic Solutions with a Unified Integral Equation Method:â€‰ Theoretical Bases, Computational Implementation, and Numerical Applications. Journal of Physical Chemistry B, 1997, 101, 10506-10517.	2.6	1,881
6	Ab initio study of ionic solutions by a polarizable continuum dielectric model. Chemical Physics Letters, 1998, 286, 253-260.	2.6	1,493
7	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	1.9	1,449
8	Geometries and properties of excited states in the gas phase and in solution: Theory and application of a time-dependent density functional theory polarizable continuum model. Journal of Chemical Physics, 2006, 124, 094107.	3.0	1,143
9	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	1.9	856
10	Polarizable continuum model. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 386-404.	14.6	679
11	Polarizable Continuum Model (PCM) Calculations of Solvent Effects on Optical Rotations of Chiral Molecules. Journal of Physical Chemistry A, 2002, 106, 6102-6113.	2.5	607
12	Fast Evaluation of Geometries and Properties of Excited Molecules in Solution:Â A Tamm-Dancoff Model with Application to 4-Dimethylaminobenzonitrile. Journal of Physical Chemistry A, 2000, 104, 5631-5637.	2.5	541
13	Formation and relaxation of excited states in solution: A new time dependent polarizable continuum model based on time dependent density functional theory. Journal of Chemical Physics, 2006, 124, 124520.	3.0	484
14	Title is missing!. Journal of Mathematical Chemistry, 1998, 23, 309-326.	1.5	422
15	Recent Advances in the Description of Solvent Effects with the Polarizable Continuum Model. Advances in Quantum Chemistry, 1998, 32, 227-261.	0.8	411
16	TD-DFT Assessment of Functionals for Optical 0â€“0 Transitions in Solvated Dyes. Journal of Chemical Theory and Computation, 2012, 8, 2359-2372.	5.3	403
17	What is Solvatochromism?. Journal of Physical Chemistry B, 2010, 114, 17128-17135.	2.6	389
18	Excited states and solvatochromic shifts within a nonequilibrium solvation approach: A new formulation of the integral equation formalism method at the self-consistent field, configuration interaction, and multiconfiguration self-consistent field level. Journal of Chemical Physics, 1998, 109, 2798-2807.	3.0	366

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19	On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. Journal of Chemical Theory and Computation, 2013, 9, 3118-3126.	5.3	335
20	Linear response theory for the polarizable continuum model. Journal of Chemical Physics, 1999, 110, 9877-9886.	3.0	313
21	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. Physical Chemistry Chemical Physics, 2011, 13, 16987.	2.8	301
22	Molecular properties in solution described with a continuum solvation model. Physical Chemistry Chemical Physics, 2002, 4, 5697-5712.	2.8	277
23	Electronic excitation energies of molecules in solution: State specific and linear response methods for nonequilibrium continuum solvation models. Journal of Chemical Physics, 2005, 122, 104513.	3.0	271
24	Quantum Chemical Studies of Light Harvesting. Chemical Reviews, 2017, 117, 294-343.	47.7	262
25	Electronic Energy Transfer in Condensed Phase Studied by a Polarizable QM/MM Model. Journal of Chemical Theory and Computation, 2009, 5, 1838-1848.	5.3	259
26	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. Journal of Chemical Theory and Computation, 2013, 9, 2749-2760.	5.3	243
27	Second-Order MÃ¸llerâ"Plesset Analytical Derivatives for the Polarizable Continuum Model Using the Relaxed Density Approach. Journal of Physical Chemistry A, 1999, 103, 9100-9108.	2.5	230
28	Self-Consistent-Field Calculation of Pauli Repulsion and Dispersion Contributions to the Solvation Free Energy in the Polarizable Continuum Model. Journal of Physical Chemistry B, 1997, 101, 1051-1057.	2.6	226
29	Practical computation of electronic excitation in solution: vertical excitation model. Chemical Science, 2011, 2, 2143.	7.4	202
30	The ONIOM-PCM method: Combining the hybrid molecular orbital method and the polarizable continuum model for solvation. Application to the geometry and properties of a merocyanine in solution. Journal of Chemical Physics, 2001, 115, 62-72.	3.0	189
31	Electronic excitation energies of molecules in solution within continuum solvation models: Investigating the discrepancy between state-specific and linear-response methods. Journal of Chemical Physics, 2005, 123, 134512.	3.0	187
32	Excitation energy transfer (EET) between molecules in condensed matter: A novel application of the polarizable continuum model (PCM). Journal of Chemical Physics, 2004, 120, 7029-7040.	3.0	184
33	Structures and Properties of Electronically Excited Chromophores in Solution from the Polarizable Continuum Model Coupled to the Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 3009-3020.	2.5	173
34	On the Performance of Continuum Solvation Methods. A Comment on â€œUniversal Approaches to Solvation Modelingâ€• Accounts of Chemical Research, 2009, 42, 489-492.	15.6	171
35	How Solvent Controls Electronic Energy Transfer and Light Harvesting. Journal of Physical Chemistry B, 2007, 111, 6978-6982.	2.6	167
36	Comment on â€œReaction field treatment of charge penetrationâ€•[J. Chem. Phys. 112, 5558 (2000)]. Journal of Chemical Physics, 2001, 114, 4744.	3.0	153

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37	Delocalized excitons in natural light-harvesting complexes. Reviews of Modern Physics, 2018, 90, .	45.6	150
38	Analytical Hartreeâ€“Fock calculation of the dynamical polarizabilities Î±, Î², and Î³ of molecules in solution. Journal of Chemical Physics, 1996, 105, 10556-10564.	3.0	149
39	Fluorescence Enhancement of Chromophores Close to Metal Nanoparticles. Optimal Setup Revealed by the Polarizable Continuum Model. Journal of Physical Chemistry C, 2009, 113, 121-133.	3.1	141
40	A QM/MM Approach Using the AMOEBA Polarizable Embedding: From Ground State Energies to Electronic Excitations. Journal of Chemical Theory and Computation, 2016, 12, 3654-3661.	5.3	136
41	Continuum Solvation Models: What Else Can We Learn from Them?. Journal of Physical Chemistry Letters, 2010, 1, 1666-1674.	4.6	134
42	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. Physical Chemistry Chemical Physics, 2010, 12, 8016.	2.8	126
43	A variational formulation of the polarizable continuum model. Journal of Chemical Physics, 2010, 133, 014106.	3.0	125
44	Theoretical Study of the Photophysics of Adenine in Solution:Â Tautomerism, Deactivation Mechanisms, and Comparison with the 2-Aminopurine Fluorescent Isomer. Journal of Physical Chemistry A, 2001, 105, 4749-4757.	2.5	123
45	Photosynthetic Light-Harvesting Is Tuned by the Heterogeneous Polarizable Environment of the Protein. Journal of the American Chemical Society, 2011, 133, 3078-3084.	13.7	123
46	Benchmarking Time-Dependent Density Functional Theory for Excited State Geometries of Organic Molecules in Gas-Phase and in Solution. Journal of Chemical Theory and Computation, 2013, 9, 2209-2220.	5.3	123
47	An integrated effective fragmentâ€”polarizable continuum approach to solvation: Theory and application to glycine. Journal of Chemical Physics, 2002, 116, 5023.	3.0	120
48	An Attempt To Bridge the Gap between Computation and Experiment for Nonlinear Optical Properties:Â Macroscopic Susceptibilities in Solutionâ€. Journal of Physical Chemistry A, 2000, 104, 4690-4698.	2.5	118
49	Fretting about FRET: Failure of the Ideal Dipole Approximation. Biophysical Journal, 2009, 96, 4779-4788.	0.5	118
50	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.	2.6	117
51	Analytical free energy second derivatives with respect to nuclear coordinates: Complete formulation for electrostatic continuum solvation models. Journal of Chemical Physics, 1999, 110, 6858-6870.	3.0	115
52	Modulation of the Optical Response of Polyethylene Films Containing Luminescent Perylene Chromophores. Journal of Physical Chemistry B, 2008, 112, 3668-3679.	2.6	115
53	On the Calculation of Local Field Factors for Microscopic Static Hyperpolarizabilities of Molecules in Solution with the Aid of Quantum-Mechanical Methods. Journal of Physical Chemistry A, 1998, 102, 870-875.	2.5	114
54	Multiconfigurational self-consistent field linear response for the polarizable continuum model: Theory and application to ground and excited-state polarizabilities of para-nitroaniline in solution. Journal of Chemical Physics, 2003, 119, 5818-5827.	3.0	113

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55	Solvent Effects on Nuclear Shieldings:Â Continuum or Discrete Solvation Models To Treat Hydrogen Bond and Polarity Effects?. Journal of Physical Chemistry A, 2001, 105, 7287-7296.	2.5	112
56	Electronic Excitations in Solution: The Interplay between State Specific Approaches and a Time-Dependent Density Functional Theory Description. Journal of Chemical Theory and Computation, 2015, 11, 5782-5790.	5.3	112
57	Polarizable embedding QM/MM: the future gold standard for complex (bio)systems?. Physical Chemistry Chemical Physics, 2020, 22, 14433-14448.	2.8	109
58	Medium effects on the properties of chemical systems: An overview of recent formulations in the polarizable continuum model (PCM). International Journal of Quantum Chemistry, 1999, 75, 783-803.	2.0	108
59	Analytical derivatives for geometry optimization in solvation continuum models. I. Theory. Journal of Chemical Physics, 1998, 109, 249-259.	3.0	106
60	Nuclear magnetic shieldings in solution: Gauge invariant atomic orbital calculation using the polarizable continuum model. Journal of Chemical Physics, 1999, 110, 7627-7638.	3.0	106
61	Modeling solvent effects on chiroptical properties. Chirality, 2011, 23, 717-729.	2.6	106
62	Analytical first derivatives of molecular surfaces with respect to nuclear coordinates. Journal of Computational Chemistry, 1996, 17, 57-73.	3.3	102
63	Solvent Effects on Linear and Nonlinear Optical Properties of Donorâ^'Acceptor Polyenes:â€‰Investigation of Electronic and Vibrational Components in Terms of Structure and Charge Distribution Changes. Journal of the American Chemical Society, 1998, 120, 8834-8847.	13.7	101
64	Hydrogen Bond versus Polar Effects:Â An Ab Initio Analysis on n â†' Ï€* Absorption Spectra and N Nuclear Shieldings of Diazines in Solution. Journal of the American Chemical Society, 2002, 124, 1506-1515.	13.7	98
65	Modeling environment effects on spectroscopies through QM/classical models. Physical Chemistry Chemical Physics, 2013, 15, 6583.	2.8	96
66	Prediction of optical rotation using density functional theory: 6,8-dioxabicyclo[3.2.1]octanes. Tetrahedron: Asymmetry, 2000, 11, 2443-2448.	1.8	94
67	Analytical derivatives for geometry optimization in solvation continuum models. II. Numerical applications. Journal of Chemical Physics, 1998, 109, 260-266.	3.0	93
68	Ab Initio Study of the Electronic Excited States in 4-(N,N-Dimethylamino)benzonitrile with Inclusion of Solvent Effects:Â The Internal Charge Transfer Process. Journal of the American Chemical Society, 2000, 122, 10621-10630.	13.7	93
69	Glycine and alanine: a theoretical study of solvent effects upon energetics and molecular response properties. Computational and Theoretical Chemistry, 2000, 500, 113-127.	1.5	92
70	How to Model Solvation of Peptides? Insights from a Quantum-mechanical and Molecular Dynamics Study ofN-Methylacetamide. 1. Geometries, Infrared, and Ultraviolet Spectra in Water. Journal of Physical Chemistry B, 2005, 109, 9818-9829.	2.6	91
71	Toward a Molecular Scale Interpretation of Excitation Energy Transfer in Solvated Bichromophoric Systems. Journal of the American Chemical Society, 2005, 127, 16733-16744.	13.7	85
72	Vibrational Circular Dichroism within the Polarizable Continuum Model:Â A Theoretical Evidence of Conformation Effects and Hydrogen Bonding for (S)-(â^')-3-Butyn-2-ol in CCl4Solution. Journal of Physical Chemistry A, 2002, 106, 12331-12339.	2.5	83

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73	Theoretical Study of Guanine from Gas Phase to Aqueous Solution:â€‰ Role of Tautomerism and Its Implications in Absorption and Emission Spectra. Journal of Physical Chemistry A, 2001, 105, 7126-7134.	2.5	82
74	Fast Domain Decomposition Algorithm for Continuum Solvation Models: Energy and First Derivatives. Journal of Chemical Theory and Computation, 2013, 9, 3637-3648.	5.3	81
75	Perspective: Polarizable continuum models for quantum-mechanical descriptions. Journal of Chemical Physics, 2016, 144, 160901.	3.0	81
76	Hybrid QM/MM Molecular Dynamics with AMOEBA Polarizable Embedding. Journal of Chemical Theory and Computation, 2017, 13, 4025-4033.	5.3	81
77	Charge transfer from the carotenoid can quench chlorophyll excitation in antenna complexes of plants. Nature Communications, 2020, 11, 662.	12.8	81
78	Multiscale modelling of photoinduced processes in composite systems. Nature Reviews Chemistry, 2019, 3, 315-330.	30.2	78
79	Radiative and nonradiative decay rates of a molecule close to a metal particle of complex shape. Journal of Chemical Physics, 2004, 121, 10190-10202.	3.0	77
80	A Subsystem TDDFT Approach for Solvent Screening Effects on Excitation Energy Transfer Couplings. Journal of Chemical Theory and Computation, 2010, 6, 1843-1851.	5.3	77
81	On the TD-DFT Accuracy in Determining Single and Double Bonds in Excited-State Structures of Organic Molecules. Journal of Physical Chemistry A, 2010, 114, 13402-13410.	2.5	76
82	The effects of solvation in the theoretical spectra of cationic dyes. Theoretical Chemistry Accounts, 2005, 113, 274-280.	1.4	74
83	Quantum Chemical Modeling of the Photoinduced Activity of Multichromophoric Biosystems. Chemical Reviews, 2019, 119, 9361-9380.	47.7	73
84	A second-order, quadratically convergent multiconfigurational self-consistent field polarizable continuum model for equilibrium and nonequilibrium solvation. Journal of Chemical Physics, 2002, 117, 13-26.	3.0	71
85	Environmental Effects on the Spectroscopic Properties of Gallic Acid:â€‰ A Combined Classical and Quantum Mechanical Study. Journal of Physical Chemistry A, 2005, 109, 1933-1943.	2.5	71
86	A Quantum Chemical Interpretation of Two-Dimensional Electronic Spectroscopy of Light-Harvesting Complexes. Journal of the American Chemical Society, 2017, 139, 7558-7567.	13.7	71
87	Ab Initio Calculations of17O NMR-Chemical Shifts for Water. The Limits of PCM Theory and the Role of Hydrogen-Bond Geometry and Cooperativity. Journal of Physical Chemistry A, 2004, 108, 5851-5863.	2.5	70
88	Nonequilibrium formulation of infrared frequencies and intensities in solution: Analytical evaluation within the polarizable continuum model. Journal of Chemical Physics, 2000, 113, 11270-11279.	3.0	69
89	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.	5.3	69
90	Solvent Effects on the Indirect Spinâ€“Spin Coupling Constants of Benzene: The DFT-PCM Approach. International Journal of Molecular Sciences, 2003, 4, 119-134.	4.1	68

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91	Nonsymmetric bent-core liquid crystals based on a 1,3,4-thiadiazole core unit and their nematic mesomorphism. Chemistry of Materials, 2011, 23, 2630-2636.	6.7	67
92	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.	2.6	65
93	How the Environment Controls Absorption and Fluorescence Spectra of PRODAN:â€‰ A Quantum-Mechanical Study in Homogeneous and Heterogeneous Media. Journal of Physical Chemistry B, 2008, 112, 414-423.	2.6	65
94	The Fennaâ€“Matthewsâ€“Olson Protein Revisited: A Fully Polarizable (TD)DFT/MM Description. ChemPhysChem, 2014, 15, 3194-3204.	2.1	65
95	Chromophoreâ€–Protein Coupling beyond Nonpolarizable Models: Understanding Absorption in Green Fluorescent Protein. Journal of Chemical Theory and Computation, 2015, 11, 4825-4839.	5.3	65
96	Correction of cavity-induced errors in polarization charges of continuum solvation models. Journal of Computational Chemistry, 1998, 19, 833-846.	3.3	64
97	Calculation and analysis of the harmonic vibrational frequencies in molecules at extreme pressure: Methodology and diborane as a test case. Journal of Chemical Physics, 2012, 137, 154112.	3.0	64
98	An Ab Initio Description of the Excitonic Properties of LH2 and Their Temperature Dependence. Journal of Physical Chemistry B, 2016, 120, 11348-11359.	2.6	64
99	MCSCF Study of the SN2 Menshutkin Reaction in Aqueous Solution within the Polarizable Continuum Model. Journal of Physical Chemistry B, 1998, 102, 3023-3028.	2.6	62
100	A time-dependent polarizable continuum model: Theory and application. Journal of Chemical Physics, 2005, 122, 154501.	3.0	62
101	How to Model Solvent Effects on Molecular Properties Using Quantum Chemistry? Insights from Polarizable Discrete or Continuum Solvation Models. Journal of Physical Chemistry A, 2007, 111, 9890-9900.	2.5	62
102	Ultrafast light harvesting dynamics in the cryptophyte phycocyanin 645. Photochemical and Photobiological Sciences, 2007, 6, 964-975.	2.9	62
103	Towards the elaboration of a QM method to describe molecular solutes under the effect of a very high pressure. Chemical Physics, 2008, 344, 135-141.	1.9	59
104	The role of charge-transfer states in the spectral tuning of antenna complexes of purple bacteria. Photosynthesis Research, 2018, 137, 215-226.	2.9	59
105	Solvation Dynamics in Acetonitrile:Â A Study Incorporating Solute Electronic Response and Nuclear Relaxation. Journal of Physical Chemistry B, 2005, 109, 3553-3564.	2.6	58
106	Fine control of chlorophyll-carotenoid interactions defines the functionality of light-harvesting proteins in plants. Scientific Reports, 2017, 7, 13956.	3.3	57
107	Soluteâ€”solvent electrostatic interactions with non-homogeneous radial dielectric functions. Chemical Physics Letters, 1994, 228, 165-170.	2.6	55
108	Density Functional Study of the Optical Rotation of Glucose in Aqueous Solution. Journal of Organic Chemistry, 2004, 69, 8161-8164.	3.2	55

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109	Solvent Effects on the Electronic Spectra:Â An Extension of the Polarizable Continuum Model to the ZINDO Method. Journal of Physical Chemistry A, 2004, 108, 6248-6256.	2.5	55
110	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.	2.6	55
111	Coupling to Charge Transfer States is the Key to Modulate the Optical Bands for Efficient Light Harvesting in Purple Bacteria. Journal of Physical Chemistry Letters, 2018, 9, 6892-6899.	4.6	55
112	Quantum mechanical methods applied to excitation energy transfer: A comparative analysis on excitation energies and electronic couplings. Journal of Chemical Physics, 2008, 129, 034104.	3.0	54
113	The role of the environment in electronic energy transfer: a molecular modeling perspective. Physical Chemistry Chemical Physics, 2011, 13, 11538.	2.8	53
114	Polarity-Sensitive Fluorescent Probes in Lipid Bilayers: Bridging Spectroscopic Behavior and Microenvironment Properties. Journal of Physical Chemistry B, 2011, 115, 9980-9989.	2.6	52
115	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.	5.3	52
116	Geometry Optimization in Polarizable QM/MM Models: The Induced Dipole Formulation. Journal of Chemical Theory and Computation, 2014, 10, 1588-1598.	5.3	52
117	Optical Signatures of OBO Fluorophores: A Theoretical Analysis. Journal of Chemical Theory and Computation, 2014, 10, 805-815.	5.3	52
118	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.	3.3	49
119	Energy Flow in the Cryptophyte PE545 Antenna Is Directed by Bilin Pigment Conformation. Journal of Physical Chemistry B, 2013, 117, 4263-4273.	2.6	49
120	On the Photophysics of Carotenoids: A Multireference DFT Study of Peridinin. Journal of Physical Chemistry B, 2013, 117, 13808-13815.	2.6	48
121	Electronic excitation energies in solution at equation of motion CCSD level within a state specific polarizable continuum model approach. Journal of Chemical Physics, 2010, 132, 084102.	3.0	47
122	Thiazole orange (TO) as a light-switch probe: a combined quantum-mechanical and spectroscopic study. Physical Chemistry Chemical Physics, 2011, 13, 12595.	2.8	47
123	Quantum, classical, and hybrid QM/MM calculations in solution: General implementation of the ddCOSMO linear scaling strategy. Journal of Chemical Physics, 2014, 141, 184108.	3.0	47
124	Towards an ab initio description of the optical spectra of light-harvesting antennae: application to the CP29 complex of photosystem II. Physical Chemistry Chemical Physics, 2015, 17, 14405-14416.	2.8	47
125	A quantum mechanical polarizable continuum model for the calculation of resonance Raman spectra in condensed phase. Theoretical Chemistry Accounts, 2007, 117, 1029-1039.	1.4	46
126	Surface-Enhanced Fluorescence within a Metal Nanoparticle Array: The Role of Solvent and Plasmon Couplings. Journal of Physical Chemistry C, 2011, 115, 5450-5460.	3.1	46

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127	Coherence in carotenoid-to-chlorophyll energy transfer. Nature Communications, 2018, 9, 3160.	12.8	46
128	A TDDFT/MMPol/PCM model for the simulation of exciton-coupled circular dichroism spectra. Physical Chemistry Chemical Physics, 2014, 16, 16407-16418.	2.8	45
129	Polarizable Molecular Dynamics in a Polarizable Continuum Solvent. Journal of Chemical Theory and Computation, 2015, 11, 623-634.	5.3	45
130	Classical Force Fields Tailored for QM Applications: Is It Really a Feasible Strategy?. Journal of Chemical Theory and Computation, 2017, 13, 4636-4648.	5.3	45
131	Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. Chemical Science, 2019, 10, 7200-7211.	7.4	45
132	On the effect of Pauli repulsion and dispersion on static molecular polarizabilities and hyperpolarizabilities in solution. Chemical Physics Letters, 1998, 286, 221-225.	2.6	44
133	Refinements on solvation continuum models: Hydrogen-bond effects on the OH stretch in liquid water and methanol. Journal of Chemical Physics, 2000, 112, 5382-5392.	3.0	44
134	Theoretical study of the SN2 reaction of Clâ¯(H2O)+CH3Cl using our own N-layered integrated molecular orbital and molecular mechanics polarizable continuum model method (ONIOM, PCM). Theoretical Chemistry Accounts, 2004, 111, 154-161.	1.4	44
135	An investigation of the photophysical properties of minor groove bound and intercalated DAPI through quantum-mechanical and spectroscopic tools. Physical Chemistry Chemical Physics, 2013, 15, 4596.	2.8	44
136	Carotenoids and Light-Harvesting: From DFT/MRCI to the Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2015, 11, 655-666.	5.3	44
137	A theoretical model of solvation in continuum anisotropic dielectrics. Journal of Chemical Physics, 1995, 102, 6837-6845.	3.0	43
138	The escaped charge problem in solvation continuum models. Journal of Chemical Physics, 2001, 115, 6130-6135.	3.0	43
139	Solvent polarity scales revisited: a ZINDO-PCM study of the solvatochromism of betaine-30. Molecular Physics, 2006, 104, 875-887.	1.7	43
140	Molecular basis of the excitonâ€“phonon interactions in the PE545 light-harvesting complex. Physical Chemistry Chemical Physics, 2014, 16, 16302-16311.	2.8	43
141	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.	5.3	43
142	Analysis of the Opposite Solvent Effects Caused by Different Solute Cavities on the Metalâ¯Water Distance of Monoatomic Cation Hydrates. Journal of Physical Chemistry B, 2002, 106, 1118-1123.	2.6	42
143	Combining classical molecular dynamics and quantum mechanical methods for the description of electronic excitations: The case of carotenoids. Journal of Computational Chemistry, 2016, 37, 981-991.	3.3	40
144	Probing the interactions between disulfide-based ligands and gold nanoparticles using a functionalised fluorescent perylene-monoimide dye. Photochemical and Photobiological Sciences, 2010, 9, 1042-1054.	2.9	39

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145	The Multiple Roles of the Protein in the Photoactivation of Orange Carotenoid Protein. CheM, 2020, 6, 187-203.	11.7	39
146	How to Model Solvation of Peptides? Insights from a Quantum Mechanical and Molecular Dynamics Study ofN-Methylacetamide. 2.15N and17O Nuclear Shielding in Water and in Acetone. Journal of Physical Chemistry B, 2005, 109, 9830-9838.	2.6	38
147	Solvation of Coumarin 153 in Supercritical Fluoroform. Journal of Physical Chemistry B, 2006, 110, 4953-4962.	2.6	38
148	The modeling of the absorption lineshape for embedded molecules through a polarizable QM/MM approach. Photochemical and Photobiological Sciences, 2018, 17, 552-560.	2.9	38
149	The Cottonâ€“Mouton effect of furan and its homologues in the gas phase, for the pure liquids and in solution. Journal of Chemical Physics, 2003, 118, 10712-10724.	3.0	37
150	Quantum-Mechanical Continuum Solvation Study of the Polarizability of Halides at the Water/Air Interface. Journal of Physical Chemistry B, 2004, 108, 13796-13806.	2.6	37
151	EXAT: EXcitonic analysis tool. Journal of Computational Chemistry, 2018, 39, 279-286.	3.3	37
152	Absolute Configuration of Natural Cyclohexene Oxides by Time Dependent Density Functional Theory Calculation of the Optical Rotation:â€‰ The Absolute Configuration of (â^')-Sphaeropsidone and (â^')-Episphaeropsidone Revised. Journal of Organic Chemistry, 2007, 72, 6680-6691.	3.2	36
153	Modeling absorption and fluorescence solvatochromism with <scp>QM</scp>/Classical approaches. International Journal of Quantum Chemistry, 2015, 115, 1202-1208.	2.0	36
154	Atomic Detail of Protein Folding Revealed by an Ab Initio Reappraisal of Circular Dichroism. Journal of the American Chemical Society, 2018, 140, 3674-3682.	13.7	36
155	Simple Protocol for Capturing Both Linear-Response and State-Specific Effects in Excited-State Calculations with Continuum Solvation Models. Journal of Chemical Theory and Computation, 2021, 17, 5155-5164.	5.3	36
156	Toward a General Formulation of Dispersion Effects for Solvation Continuum Models. Journal of Chemical Theory and Computation, 2010, 6, 3358-3364.	5.3	35
157	Plasmon-Controlled Light-Harvesting: Design Rules for Biohybrid Devices via Multiscale Modeling. Nano Letters, 2013, 13, 4475-4484.	9.1	35
158	Quantum mechanical calculations coupled with a dynamical continuum model for the description of dielectric relaxation: Time dependent Stokes shift of coumarin C153 in polar solvents. Journal of Molecular Liquids, 2003, 108, 21-46.	4.9	34
159	Limits and potentials of quantum chemical methods in modelling photosynthetic antennae. Physical Chemistry Chemical Physics, 2015, 17, 30783-30792.	2.8	34
160	Excited State Dipole Moments in Solution: Comparison between State-Specific and Linear-Response TD-DFT Values. Journal of Chemical Theory and Computation, 2018, 14, 1544-1553.	5.3	33
161	Superexchange-mediated electronic energy transfer in a model dyad. Physical Chemistry Chemical Physics, 2010, 12, 7378.	2.8	32
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