# Benedetta Mennucci

List of Publications by Year
in descending order



| 330 | 51,260 | 9428 76 | 1631 221 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 343 | 343 | 343 | 36042 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Multiscale strategies for describing environment effects: From solvents to biomatrices. , 2022, , 263-279. | | 0 |
| 2 | Unravelling the ultrafast dynamics of a N-BODIPY compound. Dyes and Pigments, 2022, 200, 110181. | 2.0 | 2 |
| 3 | Probing aqueous ions with non-local Auger relaxation. Physical Chemistry Chemical Physics, 2022, 24, 8661-8671. | 1.3 | 4 |
| 4 | Structure of the stress-related LHCSR1 complex determined by an integrated computational strategy. Communications Biology, 2022, 5, 145. | 2.0 | 8 |
| 5 | The atomistic modeling of light-harvesting complexes from the physical models to the computational protocol. Journal of Chemical Physics, 2022, 156, 120901. | 1.2 | 21 |
| 6 | A fast method for electronic couplings in embedded multichromophoric systems. Journal of Physics Condensed Matter, 2022, 34, 304004. | 0.7 | 7 |
| 7 | Uncovering the interactions driving carotenoid binding in light-harvesting complexes. Chemical Science, 2021, 12, 5113-5122. | 3.7 | 18 |
| 8 | The structural changes in the signaling mechanism of bacteriophytochromes in solution revealed by a multiscale computational investigation. Chemical Science, 2021, 12, 5555-5565. | 3.7 | 8 |
| 9 | Computational Investigation of Structural and Spectroscopic Properties of LOV-Based Proteins with Improved Fluorescence. Journal of Physical Chemistry B, 2021, 125, 1768-1777. | 1.2 | 6 |
| 10 | Multiscale Models for Light-Driven Processes. Annual Review of Physical Chemistry, 2021, 72, 489-513. | 4.8 | 29 |
| 11 | An enhanced sampling QM/AMOEBA approach: The case of the excited state intramolecular proton transfer in solvated 3-hydroxyflavone. Journal of Chemical Physics, 2021, 154, 184107. | 1.2 | 11 |
| 12 | Excited States of Xanthophylls Revisited: Toward the Simulation of Biologically Relevant Systems. Journal of Physical Chemistry Letters, 2021, 12, 6604-6612. | 2.1 | 13 |
| 13 | 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. | 2.3 | 36 |
| 14 | Energy, Structures, and Response Properties with a Fully Coupled QM/AMOEBA/ddCOSMO Implementation. Journal of Chemical Theory and Computation, 2021, 17, 5661-5672. | 2.3 | 8 |
| 15 | Ultrafast Transient Infrared Spectroscopy of Photoreceptors with Polarizable QM/MM Dynamics. Journal of Physical Chemistry B, 2021, 125, 10282-10292. | 1.2 | 9 |
| 16 | From crystallographic data to the solution structure of photoreceptors: the case of the AppA BLUF domain. Chemical Science, 2021, 12, 13331-13342. | 3.7 | 9 |
| 17 | Hybrid QM/classical models: Methodological advances and new applications. Chemical Physics Reviews, 2021, 2, . | 2.6 | 26 |
| 18 | A different perspective for nonphotochemical quenching in plant antenna complexes. Nature Communications, 2021, 12, 7152. | 5.8 | 22 |

| # | Article | IF | Citations |
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| 19 | Successes & challenges in the atomistic modeling of light-harvesting and its photoregulation. Biochimica Et Biophysica Acta - Bioenergetics, 2020, 1861, 148049. | 0.5 | 28 |
| 20 | The Multiple Roles of the Protein in the Photoactivation of Orange Carotenoid Protein. CheM, 2020, 6, 187-203. | 5.8 | 39 |
| 21 | Electronic couplings for photo-induced processes from subsystem time-dependent density-functional theory: The role of the diabatization. Journal of Chemical Physics, 2020, 153, 184113. | 1.2 | 12 |
| 22 | Excited state Bornâ€“Oppenheimer molecular dynamics through coupling between time dependent DFT and AMOEBA. Physical Chemistry Chemical Physics, 2020, 22, 19532-19541. | 1.3 | 19 |
| 23 | The energy transfer model of nonphotochemical quenching: Lessons from the minor CP29 antenna complex of plants. Biochimica Et Biophysica Acta - Bioenergetics, 2020, 1861, 148282. | 0.5 | 23 |
| 24 | Dye Stabilization and Wavelength Tunability in Lasing Fibers Based on DNA. Advanced Optical Materials, 2020, 8, 2001039. | 3.6 | 11 |
| 25 | Molecular Mechanisms of Activation in the Orange Carotenoid Protein Revealed by Molecular Dynamics. Journal of the American Chemical Society, 2020, 142, 21829-21841. | 6.6 | 18 |
| 26 | A polarisable QM/MM description of NMR chemical shifts of a photoreceptor protein. Molecular Physics, 2020, 118, e1771449. | 0.8 | 9 |
| 27 | Polarizable embedding QM/MM: the future gold standard for complex (bio)systems?. Physical Chemistry Chemical Physics, 2020, 22, 14433-14448. | 1.3 | 109 |
| 28 | Elucidating the role of structural fluctuations, and intermolecular and vibronic interactions in the spectroscopic response of a bacteriophytochrome. Physical Chemistry Chemical Physics, 2020, 22, 8585-8594. | 1.3 | 15 |
| 29 | Exciton properties and optical spectra of light harvesting complex II from a fully atomistic description. Physical Chemistry Chemical Physics, 2020, 22, 16783-16795. | 1.3 | 27 |
| 30 | Charge transfer from the carotenoid can quench chlorophyll excitation in antenna complexes of plants. Nature Communications, 2020, 11, 662. | 5.8 | 81 |
| 31 | The key to the yellow-to-cyan tuning in the green fluorescent protein family is polarisation. Physical Chemistry Chemical Physics, 2019, 21, 18988-18998. | 1.3 | 21 |
| 32 | The JPC Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848. | 1.1 | 2 |
| 33 | The JPC Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984. | 1.2 | 1 |
| 34 | The JPC Periodic Table. Journal of Physical Chemistry C, 2019, 123, 17063-17074. | 1.5 | 1 |
| 35 | The JPC Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062. | 2.1 | 2 |
| 36 | Coupled Cluster Theory with Induced Dipole Polarizable Embedding for Ground and Excited States. Journal of Chemical Theory and Computation, 2019, 15, 4485-4496. | 2.3 | 13 |

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| 37 | Quantum Chemical Modeling of the Photoinduced Activity of Multichromophoric Biosystems. Chemical Reviews, 2019, 119, 9361-9380. | 23.0 | 73 |
| 38 | Auramine O interaction with DNA: a combined spectroscopic and TD-DFT analysis. Physical Chemistry Chemical Physics, 2019, 21, 20606-20612. | 1.3 | 11 |
| 39 | Photoinduced electron transfer in 5-bromouracil labeled DNA. A contrathermodynamic mechanism revisited by electron transfer theories. Physical Chemistry Chemical Physics, 2019, 21, 4387-4393. | 1.3 | 9 |
| 40 | Time-Dependent Complete Active Space Embedded in a Polarizable Force Field. Journal of Chemical Theory and Computation, 2019, 15, 1633-1641. | 2.3 | 16 |
| 41 | Binding of model polycyclic aromatic hydrocarbons and carbamate-pesticides to DNA, BSA, micelles and liposomes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 223, 117313. | 2.0 | 17 |
| 42 | Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. Chemical Science, 2019, 10, 7200-7211. | 3.7 | 45 |
| 43 | Multiscale modelling of photoinduced processes in composite systems. Nature Reviews Chemistry, 2019, 3, 315-330. | 13.8 | 78 |
| 44 | Negative Solvatochromism in a N-Linked p-Pyridiniumcalix[4]arene Derivative. Organic Letters, 2019, 21, 2704-2707. | 2.4 | 7 |
| 45 | The molecular mechanisms of light adaption in light-harvesting complexes of purple bacteria revealed by a multiscale modeling. Chemical Science, 2019, 10, 9650-9662. | 3.7 | 26 |
| 46 | How to make continuum solvation incredibly fast in a few simple steps: A practical guide to the domain decomposition paradigm for the conductorâ€like screening model. International Journal of Quantum Chemistry, 2019, 119, e25669. | 1.0 | 17 |
| 47 | Electronic energy transfer in biomacromolecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1392. | 6.2 | 30 |
| 48 | A Synthetic Oxygen Sensor for Plants Based on Animal Hypoxia Signaling. Plant Physiology, 2019, 179, 986-1000. | 2.3 | 26 |
| 49 | Critical assessment of solvent effects on absorption and fluorescence of 3HF in acetonitrile in the QM/PCM framework: A synergic computational and experimental study. Journal of Molecular Structure, 2019, 1182, 283-291. | 1.8 | 10 |
| 50 | Nonequilibrium Environment Dynamics in a Frequency-Dependent Polarizable Embedding Model. Journal of Chemical Theory and Computation, 2019, 15, 43-51. | 2.3 | 24 |
| 51 | The modeling of the absorption lineshape for embedded molecules through a polarizable QM/MM approach. Photochemical and Photobiological Sciences, 2018, 17, 552-560. | 1.6 | 38 |
| 52 | Atomic Detail of Protein Folding Revealed by an Ab Initio Reappraisal of Circular Dichroism. Journal of the American Chemical Society, 2018, 140, 3674-3682. | 6.6 | 36 |
| 53 | The role of charge-transfer states in the spectral tuning of antenna complexes of purple bacteria. Photosynthesis Research, 2018, 137, 215-226. | 1.6 | 59 |
| 54 | The Dynamic Origin of Color Tuning in Proteins Revealed by a Carotenoid Pigment. Journal of Physical Chemistry Letters, 2018, 9, 2404-2410. | 2.1 | 26 |

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| 55 | Frenkelâ€exciton decomposition analysis of circular dichroism and circularly polarized luminescence for multichromophoric systems. Journal of Computational Chemistry, 2018, 39, 931-935. | 1.5 | 9 |
| 56 | 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 |
| 57 | 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. | 2.3 | 33 |
| 58 | Electron and excitation energy transfers in covalently linked donorâ€“acceptor dyads: mechanisms and dynamics revealed using quantum chemistry. Physical Chemistry Chemical Physics, 2018, 20, 395-403. | 1.3 | 10 |
| 59 | Polarizable QM/Classical Approaches for the Modeling of Solvation Effects on UVâ€“Vis and Fluorescence Spectra: An Integrated Strategy. Journal of Physical Chemistry A, 2018, 122, 390-397. | 1.1 | 20 |
| 60 | Modelling excitation energy transfer in covalently linked molecular dyads containing a BODIPY unit and a macrocycle. Physical Chemistry Chemical Physics, 2018, 20, 1993-2008. | 1.3 | 12 |
| 61 | EXAT: EXcitonic analysis tool. Journal of Computational Chemistry, 2018, 39, 279-286. | 1.5 | 37 |
| 62 | 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. | 2.1 | 55 |
| 63 | Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. Journal of Chemical Theory and Computation, 2018, 14, 6139-6148. | 2.3 | 29 |
| 64 | Coherence in carotenoid-to-chlorophyll energy transfer. Nature Communications, 2018, 9, 3160. | 5.8 | 46 |
| 65 | Understanding the influence of disorder on the exciton dynamics and energy transfer in Zn-phthalocyanine H-aggregates. Physical Chemistry Chemical Physics, 2018, 20, 22331-22341. | 1.3 | 9 |
| 66 | Delocalized excitons in natural light-harvesting complexes. Reviews of Modern Physics, 2018, 90, . | 16.4 | 150 |
| 67 | A polarizable QM/MM description of environment effects on NMR shieldings: from solvated molecules to pigmentâ€“protein complexes. Theoretical Chemistry Accounts, 2018, 137, 1. | 0.5 | 8 |
| 68 | Shaping excitons in light-harvesting proteins through nanoplasmonics. Chemical Science, 2018, 9, 6219-6227. | 3.7 | 9 |
| 69 | Quantum Chemical Studies of Light Harvesting. Chemical Reviews, 2017, 117, 294-343. | 23.0 | 262 |
| 70 | Fluorescent dyes in the context of DNAâ€binding: The case of Thioflavin T. International Journal of Quantum Chemistry, 2017, 117, e25349. | 1.0 | 13 |
| 71 | Modeling excitation energy transfer in multi-BODIPY architectures. Physical Chemistry Chemical Physics, 2017, 19, 6443-6453. | 1.3 | 16 |
| 72 | 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 |

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| 73 | Excited state characterization of carbonyl containing carotenoids: a comparison between single and multireference descriptions. Physical Chemistry Chemical Physics, 2017, 19, 17156-17166. | 1.3 | 15 |
| 74 | A Quantum Chemical Interpretation of Two-Dimensional Electronic Spectroscopy of Light-Harvesting Complexes. Journal of the American Chemical Society, 2017, 139, 7558-7567. | 6.6 | 71 |
| 75 | Excited state gradients for a state-specific continuum solvation approach: The vertical excitation model within a Lagrangian TDDFT formulation. Journal of Chemical Physics, 2017, 146, 204106. | 1.2 | 26 |
| 76 | A quantum chemical investigation of the solvatochromism of a phthalocyanine within a lipid bilayer: Comparison between continuum and atomistic models. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 344, 42-48. | 2.0 | 4 |
| 77 | The JPCL New Yearâ€™s Editorial. Journal of Physical Chemistry Letters, 2017, 8, 41-41. | 2.1 | 0 |
| 78 | Is energy transfer limiting multiphotochromism? answers from ab initio quantifications. Physical Chemistry Chemical Physics, 2017, 19, 2044-2052. | 1.3 | 11 |
| 79 | Fine control of chlorophyll-carotenoid interactions defines the functionality of light-harvesting proteins in plants. Scientific Reports, 2017, 7, 13956. | 1.6 | 57 |
| 80 | Exciton transport in the PE545 complex: insight from atomistic QM/MM-based quantum master equations and elastic network models. Physical Biology, 2017, 14, 066001. | 0.8 | 4 |
| 81 | Coupling Real-Time Time-Dependent Density Functional Theory with Polarizable Force Field. Journal of Physical Chemistry Letters, 2017, 8, 5283-5289. | 2.1 | 25 |
| 82 | Solvatation als Ursache fÃ¼r die unerwartete Nucleophilieâ€Reihung von Peroxidâ€Anionen. Angewandte Chemie, 2017, 129, 13463-13467. | 1.6 | 6 |
| 83 | Classical Force Fields Tailored for QM Applications: Is It Really a Feasible Strategy?. Journal of Chemical Theory and Computation, 2017, 13, 4636-4648. | 2.3 | 45 |
| 84 | Hybrid QM/MM Molecular Dynamics with AMOEBA Polarizable Embedding. Journal of Chemical Theory and Computation, 2017, 13, 4025-4033. | 2.3 | 81 |
| 85 | Solvation Accounts for the Counterintuitive Nucleophilicity Ordering of Peroxide Anions. Angewandte Chemie - International Edition, 2017, 56, 13279-13282. | 7.2 | 20 |
| 86 | In the Limelight. Journal of Physical Chemistry Letters, 2017, 8, 3718-3719. | 2.1 | 0 |
| 87 | Excited-State Gradients in Polarizable QM/MM Models: An Induced Dipole Formulation. Journal of Chemical Theory and Computation, 2017, 13, 3778-3786. | 2.3 | 23 |
| 88 | Noncovalent Interactions and Environment Effects. , 2017, , 365-385. | | 1 |
| 89 | 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. | 1.5 | 40 |
| 90 | Efficient Photoinduced Charge Separation in a BODIPYâ€“C<sub>60</sub> Dyad. Journal of Physical Chemistry C, 2016, 120, 16526-16536. | 1.5 | 25 |

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| 91 | Perspective: Polarizable continuum models for quantum-mechanical descriptions. Journal of Chemical Physics, 2016, 144, 160901. | 1.2 | 81 |
| 92 | Control of Coherences and Optical Responses of Pigmentâ€“Protein Complexes by Plasmonic Nanoantennae. Journal of Physical Chemistry Letters, 2016, 7, 2189-2196. | 2.1 | 14 |
| 93 | Photoprotection and triplet energy transfer in higher plants: the role of electronic and nuclear fluctuations. Physical Chemistry Chemical Physics, 2016, 18, 11288-11296. | 1.3 | 21 |
| 94 | Simulation of Electronic Circular Dichroism of Nucleic Acids: From the Structure to the Spectrum. Chemistry - A European Journal, 2016, 22, 17011-17019. | 1.7 | 28 |
| 95 | Theoretical Quantification of the Modified Photoactivity of Photochromes Grafted on Metallic Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 21827-21836. | 1.5 | 6 |
| 96 | Excited-State Decay Pathways of Molecular Rotors: Twisted Intermediate or Conical Intersection?. Journal of Physical Chemistry Letters, 2016, 7, 4285-4290. | 2.1 | 28 |
| 97 | Electrostatic versus Resonance Interactions in Photoreceptor Proteins: The Case of Rhodopsin. Journal of Physical Chemistry Letters, 2016, 7, 4547-4553. | 2.1 | 25 |
| 98 | An Ab Initio Description of the Excitonic Properties of LH2 and Their Temperature Dependence. Journal of Physical Chemistry B, 2016, 120, 11348-11359. | 1.2 | 64 |
| 99 | 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. | 2.3 | 136 |
| 100 | Introducing QMC/MMpol: Quantum Monte Carlo in Polarizable Force Fields for Excited States. Journal of Chemical Theory and Computation, 2016, 12, 1674-1683. | 2.3 | 28 |
| 101 | Reaching Out with Physical Chemistry. Journal of Physical Chemistry Letters, 2016, 7, 103-104. | 2.1 | 1 |
| 102 | A fast but accurate excitonic simulation of the electronic circular dichroism of nucleic acids: how can it be achieved?. Physical Chemistry Chemical Physics, 2016, 18, 866-877. | 1.3 | 24 |
| 103 | Modeling absorption and fluorescence solvatochromism with <scp>QM</scp>/Classical approaches. International Journal of Quantum Chemistry, 2015, 115, 1202-1208. | 1.0 | 36 |
| 104 | FemExâ€”female excellence in theoretical and computational chemistry. International Journal of Quantum Chemistry, 2015, 115, 1195-1196. | 1.0 | 3 |
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| 106 | Carotenoids and Light-Harvesting: From DFT/MRCI to the Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2015, 11, 655-666. | 2.3 | 44 |
| 107 | Polarizable Molecular Dynamics in a Polarizable Continuum Solvent. Journal of Chemical Theory and Computation, 2015, 11, 623-634. | 2.3 | 45 |
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| 109 | Excited-State Vibrations of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2015, 11, 847-850. | 2.3 | 18 |
| 110 | The role of magneticâ€“electric coupling in exciton-coupled ECD spectra: the case of bis-phenanthrenes. Chemical Communications, 2015, 51, 10498-10501. | 2.2 | 32 |
| 111 | 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. | 1.3 | 47 |
| 112 | Limits and potentials of quantum chemical methods in modelling photosynthetic antennae. Physical Chemistry Chemical Physics, 2015, 17, 30783-30792. | 1.3 | 34 |
| 113 | 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 |
| 114 | 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. | 2.3 | 112 |
| 115 | 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 |
| 116 | Time-dependent non-equilibrium dielectric response in QM/continuum approaches. Journal of Chemical Physics, 2015, 142, 034120. | 1.2 | 31 |
| 117 | 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 |
| 118 | Negative solvatochromism of pushâ€“pull biphenyl compounds: a theoretical study. Theoretical Chemistry Accounts, 2015, 134, 1. | 0.5 | 6 |
| 119 | Electronic Excitations in Nonpolar Solvents: Can the Polarizable Continuum Model Accurately Reproduce Solvent Effects?. Journal of Physical Chemistry B, 2015, 119, 8984-8991. | 1.2 | 23 |
| 120 | QM/MM Approaches for the Modeling of Photoinduced Processes in Biological Systems. Challenges and Advances in Computational Chemistry and Physics, 2015, , 325-342. | 0.6 | 1 |
| 121 | Liquid-Phase Simulation: Theory and Numerics of Hybrid Quantum-Mechanical/Classical Approaches. , 2015, , 811-817. | | 0 |
| 122 | Combined Experimental and Theoretical Study of Efficient and Ultrafast Energy Transfer in a Molecular Dyad. Journal of Physical Chemistry C, 2014, 118, 23476-23486. | 1.5 | 29 |
| 123 | Geometry Optimization in Polarizable QM/MM Models: The Induced Dipole Formulation. Journal of Chemical Theory and Computation, 2014, 10, 1588-1598. | 2.3 | 52 |
| 124 | Excited-State Geometries of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2014, 10, 1848-1851. | 2.3 | 29 |
| 125 | Freezing of Molecular Motions Probed by Cryogenic Magic Angle Spinning NMR. Journal of Physical Chemistry Letters, 2014, 5, 512-516. | 2.1 | 15 |
| 126 | Optical Signatures of OBO Fluorophores: A Theoretical Analysis. Journal of Chemical Theory and Computation, 2014, 10, 805-815. | 2.3 | 52 |

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| 127 | Full cLR-PCM calculations of the solvatochromic effects on emission energies. Physical Chemistry Chemical Physics, 2014, 16, 26024-26029. | 1.3 | 13 |
| 128 | A TDDFT/MMPol/PCM model for the simulation of exciton-coupled circular dichroism spectra. Physical Chemistry Chemical Physics, 2014, 16, 16407-16418. | 1.3 | 45 |
| 129 | Molecular basis of the excitonâ€“phonon interactions in the PE545 light-harvesting complex. Physical Chemistry Chemical Physics, 2014, 16, 16302-16311. | 1.3 | 43 |
| 130 | Unveiling Solvents Effect on Excited-State Polarizabilities with the Corrected Linear-Response Model. Journal of Physical Chemistry A, 2014, 118, 5652-5656. | 1.1 | 12 |
| 131 | Excitation Energy Transfer in Donor-Bridge-Acceptor Systems: A Combined Quantum-Mechanical/Classical Analysis of the Role of the Bridge and the Solvent. Journal of Physical Chemistry A, 2014, 118, 6484-6491. | 1.1 | 17 |
| 132 | Solvation at Surfaces and Interfaces: A Quantum-Mechanical/Continuum Approach Including Nonelectrostatic Contributions. Journal of Physical Chemistry C, 2014, 118, 4715-4725. | 1.5 | 20 |
| 133 | Solvent Effects on Cyanine Derivatives: A PCM Investigation. Journal of Physical Chemistry A, 2014, 118, 5343-5348. | 1.1 | 29 |
| 134 | A Theoretical and Experimental Investigation of the Spectroscopic Properties of a DNAâ€Intercalator Salphenâ€Type Zn<sup>II</sup> Complex. Chemistry - A European Journal, 2014, 20, 7439-7447. | 1.7 | 23 |
| 135 | The Fennaâ€“Matthewsâ€“Olson Protein Revisited: A Fully Polarizable (TD)DFT/MM Description. ChemPhysChem, 2014, 15, 3194-3204. | 1.0 | 65 |
| 136 | Orientational Order of Two Fluoro- and Isothiocyanate-Substituted Nematogens by Combination of <sup>13</sup>C NMR Spectroscopy and DFT Calculations. Journal of Physical Chemistry B, 2014, 118, 3469-3477. | 1.2 | 2 |
| 137 | Quantum Calculations in Solution for Large to Very Large Molecules: A New Linear Scaling QM/Continuum Approach. Journal of Physical Chemistry Letters, 2014, 5, 953-958. | 2.1 | 32 |
| 138 | Quantum, classical, and hybrid QM/MM calculations in solution: General implementation of the ddCOSMO linear scaling strategy. Journal of Chemical Physics, 2014, 141, 184108. | 1.2 | 47 |
| 139 | Plasmon-Controlled Light-Harvesting: Design Rules for Biohybrid Devices via Multiscale Modeling. Nano Letters, 2013, 13, 4475-4484. | 4.5 | 35 |
| 140 | Conformational Analysis of Glyâ€“Alaâ€“NHMe in D<sub>2</sub>O and DMSO Solutions: A Two-Dimensional Infrared Spectroscopy Study. Journal of Physical Chemistry B, 2013, 117, 14226-14237. | 1.2 | 9 |
| 141 | On the Photophysics of Carotenoids: A Multireference DFT Study of Peridinin. Journal of Physical Chemistry B, 2013, 117, 13808-13815. | 1.2 | 48 |
| 142 | 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 |
| 143 | Can we control the electronic energy transfer in molecular dyads through metal nanoparticles? A QM/continuum investigation. Physical Chemistry Chemical Physics, 2013, 15, 3294. | 1.3 | 18 |
| 144 | Modeling environment effects on spectroscopies through QM/classical models. Physical Chemistry Chemical Physics, 2013, 15, 6583. | 1.3 | 96 |

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| 145 | Spatial and Electronic Correlations in the PE545 Light-Harvesting Complex. Journal of Physical Chemistry Letters, 2013, 4, 372-377. | 2.1 | 24 |
| 146 | Modeling Fluorescence Observables, Particularly for FRET Experiments, using Markov Chain Analysis of Molecular Dynamics and Quantum Mechanics Simulations. Biophysical Journal, 2013, 104, 683a. | 0.2 | 0 |
| 147 | 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. | 1.3 | 44 |
| 148 | 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. | 2.3 | 123 |
| 149 | Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. Journal of Chemical Theory and Computation, 2013, 9, 2749-2760. | 2.3 | 243 |
| 150 | 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 |
| 151 | Dissecting the Nature of Exciton Interactions in Ethyne-Linked Tetraarylporphyrin Arrays. Journal of Physical Chemistry C, 2013, 117, 12423-12431. | 1.5 | 6 |
| 152 | On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. Journal of Chemical Theory and Computation, 2013, 9, 3118-3126. | 2.3 | 335 |
| 153 | Fast Domain Decomposition Algorithm for Continuum Solvation Models: Energy and First Derivatives. Journal of Chemical Theory and Computation, 2013, 9, 3637-3648. | 2.3 | 81 |
| 154 | Synthesis, Chiroptical Properties and Density Functional Theory Calculations of 3,3â€™â€Biphenylâ€2,2â€™â€BiTropone. Chirality, 2013, 25, 648-655. | 1.3 | 1 |
| 155 | Modelling vibrational coupling in DNA oligomers: a computational strategy combining QM and continuum solvation models. Highlights in Theoretical Chemistry, 2013, , 143-152. | 0.0 | 0 |
| 156 | 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. | 1.2 | 64 |
| 157 | TD-DFT Assessment of Functionals for Optical 0â€“0 Transitions in Solvated Dyes. Journal of Chemical Theory and Computation, 2012, 8, 2359-2372. | 2.3 | 403 |
| 158 | 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 |
| 159 | A Photosensitive Liquid Crystal Studied by <sup>14</sup>N NMR, <sup>2</sup>H NMR, and DFT Calculations. ChemPhysChem, 2012, 13, 3958-3965. | 1.0 | 11 |
| 160 | A Strategy for the Study of the Interactions between Metalâ€“Dyes and Proteins with QM/MM Approaches: the Case of Ironâ€“Gall Dye. Journal of Physical Chemistry B, 2012, 116, 13344-13352. | 1.2 | 3 |
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