# Jacob Kongsted

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 245 papers | 8,388 citations | 50 h-index | 79 g-index |
| 251 ext. papers | 9,210 ext. citations | 4.5 avg, IF | 6.18 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 245 | Computational analysis of altered one- and two-photon CD of sterols inside a protein binding pocket. *Theoretical Chemistry Accounts*, **2022**, 141, 1 | 1.9 | |
| 244 | Importance of Ile71 in β-actin on histidine methyltransferase SETD3 catalysis.. *Organic and Biomolecular Chemistry*, **2022**, | 3.9 | 1 |
| 243 | Polarizable Embedding as a Tool to Address Light-Responsive Biological Systems. *Challenges and Advances in Computational Chemistry and Physics*, **2021**, 143-195 | 0.7 | 2 |
| 242 | Substituted 9-Diethylaminobenzo[]phenoxazin-5-ones (Nile Red Analogues): Synthesis and Photophysical Properties. *Journal of Organic Chemistry*, **2021**, 86, 1471-1488 | 4.2 | 4 |
| 241 | Efficient Open-Source Implementations of Linear-Scaling Polarizable Embedding: Use Octrees to Save the Trees. *Journal of Chemical Theory and Computation*, **2021**, 17, 3445-3454 | 6.4 | 2 |
| 240 | Harmonic Infrared and Raman Spectra in Molecular Environments Using the Polarizable Embedding Model. *Journal of Chemical Theory and Computation*, **2021**, 17, 3599-3617 | 6.4 | 2 |
| 239 | Photophysical and Structural Characterization of Intrinsically Fluorescent Sterol Aggregates. *Journal of Physical Chemistry B*, **2021**, 125, 5838-5852 | 3.4 | 1 |
| 238 | βActin Peptide-Based Inhibitors of Histidine Methyltransferase SETD3. *ChemMedChem*, **2021**, 16, 2695-2702 | 3.7 | 3 |
| 237 | Direct observation of nystatin binding to the plasma membrane of living cells. *Biochimica Et Biophysica Acta - Biomembranes*, **2021**, 1863, 183528 | 3.8 | 0 |
| 236 | Recent developments in the medicinal chemistry of single boron atom-containing compounds. *Acta Pharmaceutica Sinica B*, **2021**, 11, 3035-3059 | 15.5 | 28 |
| 235 | Preparation of organocobalt(iii) complexes via O activation. *Dalton Transactions*, **2021**, 50, 4819-4829 | 4.3 | 4 |
| 234 | Frontiers in Multiscale Modeling of Photoreceptor Proteins. *Photochemistry and Photobiology*, **2021**, 97, 243-269 | 3.6 | 8 |
| 233 | Modeling One- and Two-Photon Excitation of 4?-(Hydroxymethyl)-4,5?,8-trimethylpsoralen in Complex with DNA: Solving Electron Spill-Out Problems in Polarizable QM/MM Calculations. *Advanced Theory and Simulations*, **2021**, 4, 2000294 | 3.5 | 1 |
| 232 | Nitrogen -Edge X-ray Absorption Spectra of Ammonium and Ammonia in Water Solution: Assessing the Performance of Polarizable Embedding Coupled Cluster Methods. *Journal of Physical Chemistry Letters*, **2021**, 12, 8865-8871 | 6.4 | 5 |
| 231 | Modeling environmental effects in two-photon circular dichroism calculations. *Theoretical Chemistry Accounts*, **2021**, 140, 1 | 1.9 | 0 |
| 230 | Computational and photophysical characterization of a Laurdan malononitrile derivative. *Physical Chemistry Chemical Physics*, **2021**, 23, 9139-9146 | 3.6 | 2 |
| 229 | Fast Approximate but Accurate QM/MM Interactions for Polarizable Embedding.. *Journal of Chemical Theory and Computation*, **2021**, | 6.4 | 1 |

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| 228 | Discovery of a Potent Adenine-Benzyltriazolo-Pleuromutilin Conjugate with Pronounced Antibacterial Activity against MRSA. *Journal of Medicinal Chemistry*, **2020**, 63, 15693-15708 | 8.3 | 5 |
| 227 | Mechanistic Insight into Lipid Binding to Yeast Niemann Pick Type C2 Protein. *Biochemistry*, **2020**, 59, 4407-4420 | 3.2 | 2 |
| 226 | Modeling the Sterol-Binding Domain of Aster-A Provides Insight into Its Multiligand Specificity. *Journal of Chemical Information and Modeling*, **2020**, 60, 2268-2281 | 6.1 | 2 |
| 225 | Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. *Journal of Chemical Physics*, **2020**, 152, 214115 | 3.9 | 24 |
| 224 | Hole Hopping through Cytochrome P450. *Journal of Physical Chemistry B*, **2020**, 124, 3065-3073 | 3.4 | 2 |
| 223 | Relaxation Dynamics of the Triazene Compound Berenil in DNA-Minor-Groove Confinement after Photoexcitation. *Journal of Chemical Theory and Computation*, **2020**, 16, 5203-5211 | 6.4 | |
| 222 | Avoiding Electron Spill-Out in QM/MM Calculations on Excited States with Simple Pseudopotentials. *Journal of Chemical Theory and Computation*, **2020**, 16, 1373-1381 | 6.4 | 16 |
| 221 | Binding and intracellular transport of 25-hydroxycholesterol by Niemann-Pick C2 protein. *Biochimica Et Biophysica Acta - Biomembranes*, **2020**, 1862, 183063 | 3.8 | 7 |
| 220 | Polarizable Density Embedding for Large Biomolecular Systems. *Journal of Chemical Theory and Computation*, **2020**, 16, 5999-6006 | 6.4 | 6 |
| 219 | Membrane organization and intracellular transport of a fluorescent analogue of 27-hydroxycholesterol. *Chemistry and Physics of Lipids*, **2020**, 233, 105004 | 3.7 | 5 |
| 218 | Computational Characterization of Novel Malononitrile Variants of Laurdan with Improved Photophysical Properties for Sensing in Membranes. *Journal of Physical Chemistry B*, **2020**, 124, 9526-9534 | 3.4 | 1 |
| 217 | One- and two-photon solvatochromism of the fluorescent dye Nile Red and its CF, F and Br-substituted analogues. *Photochemical and Photobiological Sciences*, **2020**, 19, 1382-1391 | 4.2 | 6 |
| 216 | Photophysical investigation of two emissive nucleosides exhibiting gigantic stokes shifts. *Photochemical and Photobiological Sciences*, **2019**, 18, 1858-1865 | 4.2 | 2 |
| 215 | Rational design of novel fluorescent analogues of cholesterol: a "step-by-step" computational study. *Physical Chemistry Chemical Physics*, **2019**, 21, 15487-15503 | 3.6 | 5 |
| 214 | Molecular design opportunities presented by solvent-exposed regions of target proteins. *Medicinal Research Reviews*, **2019**, 39, 2194-2238 | 14.4 | 16 |
| 213 | Overview of Recent Strategic Advances in Medicinal Chemistry. *Journal of Medicinal Chemistry*, **2019**, 62, 9375-9414 | 8.3 | 53 |
| 212 | Combining polarizable embedding with the Frenkel exciton model: applications to absorption spectra with overlapping solute–solvent bands. *Theoretical Chemistry Accounts*, **2019**, 138, 1 | 1.9 | |
| 211 | Computational Characterization of a Cholesterol-Based Molecular Rotor in Lipid Membranes. *Journal of Physical Chemistry B*, **2019**, 123, 7313-7326 | 3.4 | 4 |

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| 210 | Discovery of piperidine-substituted thiazolo[5,4-d]pyrimidine derivatives as potent and orally bioavailable HIV-1 non-nucleoside reverse transcriptase inhibitors. *Communications Chemistry*, **2019**, 2, | 6.3 | 15 |
| 209 | CPPE: An Open-Source C++ and Python Library for Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2019**, 15, 6154-6163 | 6.4 | 13 |
| 208 | Rational Design of Nile Red Analogs for Sensing in Membranes. *Journal of Physical Chemistry B*, **2019**, 123, 10424-10432 | 3.4 | 5 |
| 207 | Computational Modeling Explains the Multi Sterol Ligand Specificity of the N-Terminal Domain of Niemann-Pick C1-Like 1 Protein. *ACS Omega*, **2019**, 4, 20894-20904 | 3.9 | 2 |
| 206 | Response properties of embedded molecules through the polarizable embedding model. *International Journal of Quantum Chemistry*, **2019**, 119, e25717 | 2.1 | 22 |
| 205 | Design, synthesis, and biologic evaluation of novel galloyl derivatives as HIV-1 RNase H inhibitors. *Chemical Biology and Drug Design*, **2019**, 93, 582-589 | 2.9 | 8 |
| 204 | The Journey of HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors (NNRTIs) from Lab to Clinic. *Journal of Medicinal Chemistry*, **2019**, 62, 4851-4883 | 8.3 | 74 |
| 203 | Modeling magnetic circular dichroism within the polarizable embedding approach. *Theoretical Chemistry Accounts*, **2018**, 137, 1 | 1.9 | 6 |
| 202 | Structure-guided approach identifies a novel class of HIV-1 ribonuclease H inhibitors: binding mode insights through magnesium complexation and site-directed mutagenesis studies. *MedChemComm*, **2018**, 9, 562-575 | 5 | 12 |
| 201 | Density-Dependent Formulation of Dispersion-Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. *Journal of Chemical Theory and Computation*, **2018**, 14, 1671-1681 | 6.4 | 20 |
| 200 | Polarizable Density Embedding Coupled Cluster Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 1351-1360 | 6.4 | 15 |
| 199 | Structural design of intrinsically fluorescent oxysterols. *Chemistry and Physics of Lipids*, **2018**, 212, 26-34 | 3.7 | 8 |
| 198 | One-Photon Absorption Properties from a Hybrid Polarizable Density Embedding/Complex Polarization Propagator Approach for Polarizable Solutions. *Journal of Chemical Theory and Computation*, **2018**, 14, 2145-2154 | 6.4 | 3 |
| 197 | Importance of Accurate Structures for Quantum Chemistry Embedding Methods: Which Strategy Is Better?. *Journal of Chemical Theory and Computation*, **2018**, 14, 4309-4319 | 6.4 | 19 |
| 196 | The Reaction of Oxy Hemoglobin with Nitrite: Mechanism, Antioxidant-Modulated Effect, and Implications for Blood Substitute Evaluation. *Molecules*, **2018**, 23, | 4.8 | 9 |
| 195 | Polarizable Embedding Combined with the Algebraic Diagrammatic Construction: Tackling Excited States in Biomolecular Systems. *Journal of Chemical Theory and Computation*, **2018**, 14, 4870-4883 | 6.4 | 18 |
| 194 | Absorption Spectra of FAD Embedded in Cryptochromes. *Journal of Physical Chemistry Letters*, **2018**, 9, 3618-3623 | 6.4 | 10 |
| 193 | Modeling of Magnetic Circular Dichroism and UV/Vis Absorption Spectra Using Fluctuating Charges or Polarizable Embedding within a Resonant-Convergent Response Theory Formalism. *Journal of Chemical Theory and Computation*, **2018**, 14, 6391-6404 | 6.4 | 7 |

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| 192 | Assessing frequency-dependent site polarisabilities in linear response polarisable embedding. *Molecular Physics*, **2017**, 115, 39-47 | 1.7 | 10 |
| 191 | Computational Approach to Evaluation of Optical Properties of Membrane Probes. *Journal of Chemical Theory and Computation*, **2017**, 13, 719-726 | 6.4 | 10 |
| 190 | An averaged polarizable potential for multiscale modeling in phospholipid membranes. *Journal of Computational Chemistry*, **2017**, 38, 601-611 | 3.5 | 8 |
| 189 | Very Strong Binding for a Neutral Calix[4]pyrrole Receptor Displaying Positive Allosteric Binding. *Journal of Organic Chemistry*, **2017**, 82, 2123-2128 | 4.2 | 8 |
| 188 | Optimization and transferability of non-electrostatic repulsion in the polarizable density embedding model. *Journal of Computational Chemistry*, **2017**, 38, 2108-2117 | 3.5 | 3 |
| 187 | Relativistic Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2017**, 13, 2870-2880 | 6.4 | 7 |
| 186 | Automated Fragmentation Polarizable Embedding Density Functional Theory (PE-DFT) Calculations of Nuclear Magnetic Resonance (NMR) Shielding Constants of Proteins with Application to Chemical Shift Predictions. *Journal of Chemical Theory and Computation*, **2017**, 13, 525-536 | 6.4 | 14 |
| 185 | Modeling Electronic Circular Dichroism within the Polarizable Embedding Approach. *Journal of Chemical Theory and Computation*, **2017**, 13, 4442-4451 | 6.4 | 9 |
| 184 | A quantum-mechanical perspective on linear response theory within polarizable embedding. *Journal of Chemical Physics*, **2017**, 146, 234101 | 3.9 | 11 |
| 183 | Polarizable Density Embedding: A Solution to the Electron Spill-Out Problem in Multiscale Modeling. *Journal of Physical Chemistry Letters*, **2017**, 8, 5949-5958 | 6.4 | 35 |
| 182 | The Quality of the Embedding Potential Is Decisive for Minimal Quantum Region Size in Embedding Calculations: The Case of the Green Fluorescent Protein. *Journal of Chemical Theory and Computation*, **2017**, 13, 6230-6236 | 6.4 | 22 |
| 181 | Computational Approach for Studying Optical Properties of DNA Systems in Solution. *Journal of Chemical Theory and Computation*, **2016**, 12, 5050-5057 | 6.4 | 20 |
| 180 | Computational Analysis of Sterol Ligand Specificity of the Niemann Pick C2 Protein. *Biochemistry*, **2016**, 55, 5165-79 | 3.2 | 15 |
| 179 | Excited states in large molecular systems through polarizable embedding. *Physical Chemistry Chemical Physics*, **2016**, 18, 20234-50 | 3.6 | 57 |
| 178 | Multipole moments for embedding potentials: Exploring different atomic allocation algorithms. *Journal of Computational Chemistry*, **2016**, 37, 1887-96 | 3.5 | 4 |
| 177 | How Far Does a Receptor Influence Vibrational Properties of an Odorant?. *PLoS ONE*, **2016**, 11, e0152345 | 3.7 | 12 |
| 176 | Revealing Nucleic Acid Mutations Using Förster Resonance Energy Transfer-Based Probes. *Sensors*, **2016**, 16, | 3.8 | 16 |
| 175 | Binding affinity models for Falcipain inhibition based on the Linear Interaction Energy method. *Journal of Molecular Graphics and Modelling*, **2016**, 70, 236-245 | 2.8 | 4 |

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| 174 | Embedding beyond electrostatics-The role of wave function confinement. *Journal of Chemical Physics*, **2016**, 145, 104102 | 3.9 | 17 |
| 173 | Local electric fields and molecular properties in heterogeneous environments through polarizable embedding. *Physical Chemistry Chemical Physics*, **2016**, 18, 10070-80 | 3.6 | 42 |
| 172 | Averaged Solvent Embedding Potential Parameters for Multiscale Modeling of Molecular Properties. *Journal of Chemical Theory and Computation*, **2016**, 12, 1684-95 | 6.4 | 32 |
| 171 | Open-ended response theory with polarizable embedding: multiphoton absorption in biomolecular systems. *Physical Chemistry Chemical Physics*, **2016**, 18, 28339-28352 | 3.6 | 19 |
| 170 | Molecular quantum mechanical gradients within the polarizable embedding approach--application to the internal vibrational Stark shift of acetophenone. *Journal of Chemical Physics*, **2015**, 142, 034119 | 3.9 | 15 |
| 169 | Electronic Energy Transfer in Polarizable Heterogeneous Environments: A Systematic Investigation of Different Quantum Chemical Approaches. *Journal of Chemical Theory and Computation*, **2015**, 11, 4283-93 | 6.4 | 15 |
| 168 | Benchmarking two-photon absorption cross sections: performance of CC2 and CAM-B3LYP. *Physical Chemistry Chemical Physics*, **2015**, 17, 19306-14 | 3.6 | 104 |
| 167 | Accuracy of Protein Embedding Potentials: An Analysis in Terms of Electrostatic Potentials. *Journal of Chemical Theory and Computation*, **2015**, 11, 1832-42 | 6.4 | 38 |
| 166 | Relation between Nonlinear Optical Properties of Push-Pull Molecules and Metric of Charge Transfer Excitations. *Journal of Chemical Theory and Computation*, **2015**, 11, 4182-8 | 6.4 | 32 |
| 165 | A comparative study of binding affinities for 6,7-dimethoxy-4-pyrrolidylquinazolines as phosphodiesterase 10A inhibitors using the linear interaction energy method. *Journal of Molecular Graphics and Modelling*, **2015**, 61, 44-52 | 2.8 | 3 |
| 164 | Experimental and computational study of solvent effects on one- and two-photon absorption spectra of chlorinated harmines. *Physical Chemistry Chemical Physics*, **2015**, 17, 12090-9 | 3.6 | 17 |
| 163 | Ultramild protein-mediated click chemistry creates efficient oligonucleotide probes for targeting and detecting nucleic acids. *ChemBioChem*, **2015**, 16, 1163-7 | 3.8 | 4 |
| 162 | Multiscale Modeling of the Active Site of [Fe] Hydrogenase: The H2 Binding Site in Open and Closed Protein Conformations. *Angewandte Chemie*, **2015**, 127, 6344-6348 | 3.6 | 2 |
| 161 | Multiscale modeling of the active site of [Fe] hydrogenase: the H□binding site in open and closed protein conformations. *Angewandte Chemie - International Edition*, **2015**, 54, 6246-50 | 16.4 | 18 |
| 160 | Mutations in the bacterial ribosomal protein l3 and their association with antibiotic resistance. *Antimicrobial Agents and Chemotherapy*, **2015**, 59, 3518-28 | 5.9 | 26 |
| 159 | The chemistry of Coulomb blockade diamonds for 1,4-diamino-benzene. *Chemical Physics*, **2015**, 459, 40-44 | 2.3 | 2 |
| 158 | Enhancement of Internal Motions of Lysozyme through Interaction with Gold Nanoclusters and its Optical Imaging. *Journal of Physical Chemistry C*, **2015**, 119, 653-664 | 3.8 | 15 |
| 157 | Analysis of computational models for an accurate study of electronic excitations in GFP. *Physical Chemistry Chemical Physics*, **2015**, 17, 2582-8 | 3.6 | 39 |

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| 156 | Polarizable embedding with a multiconfiguration short-range density functional theory linear response method. *Journal of Chemical Physics*, **2015**, 142, 114113 | 3.9 | 25 |
| 155 | Biochemical and Computational Analysis of the Substrate Specificities of Cfr and RlmN Methyltransferases. *PLoS ONE*, **2015**, 10, e0145655 | 3.7 | 3 |
| 154 | Design of new fluorescent cholesterol and ergosterol analogs: Insights from theory. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 2188-99 | 3.8 | 16 |
| 153 | Carotenoids and light-harvesting: from DFT/MRCI to the Tamm-Dancoff approximation. *Journal of Chemical Theory and Computation*, **2015**, 11, 655-66 | 6.4 | 37 |
| 152 | Polarizable density embedding: a new QM/QM/MM-based computational strategy. *Journal of Physical Chemistry A*, **2015**, 119, 5344-55 | 2.8 | 63 |
| 151 | Comparison between theoretically and experimentally determined electronic properties: applications to two-photon singlet oxygen sensitizers. *Journal of Physical Chemistry A*, **2015**, 119, 1906-16 | 2.8 | 2 |
| 150 | One- and two-photon absorption of a spiropyran-merocyanine system: experimental and theoretical studies. *Journal of Physical Chemistry B*, **2015**, 119, 1515-22 | 3.4 | 16 |
| 149 | The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284 | 7.9 | 956 |
| 148 | Effect of chromophore encapsulation on linear and nonlinear optical properties: the case of "miniSOG", a protein-encased flavin. *Physical Chemistry Chemical Physics*, **2014**, 16, 9950-9 | 3.6 | 19 |
| 147 | Polarizable embedding based on multiconfigurational methods: Current developments and the road ahead. *International Journal of Quantum Chemistry*, **2014**, 114, 1102-1107 | 2.1 | 10 |
| 146 | Computational assignment of redox states to Coulomb blockade diamonds. *Physical Chemistry Chemical Physics*, **2014**, 16, 17473-8 | 3.6 | 9 |
| 145 | Theoretical 57Fe Mössbauer spectroscopy: isomer shifts of [Fe]-hydrogenase intermediates. *Physical Chemistry Chemical Physics*, **2014**, 16, 4853-63 | 3.6 | 17 |
| 144 | Dual mechanism of HIV-1 integrase and RNase H inhibition by diketo derivatives – a computational study. *RSC Advances*, **2014**, 4, 38672-38681 | 3.7 | 6 |
| 143 | Binding free energy based structural dynamics analysis of HIV-1 RT RNase H-inhibitor complexes. *Integrative Biology (United Kingdom)*, **2014**, 6, 1010-22 | 3.7 | 17 |
| 142 | Promising two-photon probes for in vivo detection of β-amyloid deposits. *Chemical Communications*, **2014**, 50, 11694-7 | 5.8 | 21 |
| 141 | Simulations of light absorption of carbon particles in nanoaerosol clusters. *Journal of Physical Chemistry A*, **2014**, 118, 1879-86 | 2.8 | 6 |
| 140 | Dehydroergosterol as an analogue for cholesterol: why it mimics cholesterol so well-or does it?. *Journal of Physical Chemistry B*, **2014**, 118, 7345-57 | 3.4 | 26 |
| 139 | Self-aggregation and optical absorption of stilbazolium merocyanine in chloroform. *Journal of Physical Chemistry B*, **2014**, 118, 1715-25 | 3.4 | 16 |

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| 138 | Basis set error estimation for DFT calculations of electronic g-tensors for transition metal complexes. *Journal of Computational Chemistry*, **2014**, 35, 1809-14 | 3.5 | 3 |
| 137 | Damped Response Theory in Combination with Polarizable Environments: The Polarizable Embedding Complex Polarization Propagator Method. *Journal of Chemical Theory and Computation*, **2014**, 10, 1164-71 | 6.4 | 40 |
| 136 | Convergence of environment polarization effects in multiscale modeling of excitation energies. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 304-311 | 2 | 29 |
| 135 | Nuclear Magnetic Shielding Constants from Quantum Mechanical/Molecular Mechanical Calculations Using Polarizable Embedding: Role of the Embedding Potential. *Journal of Chemical Theory and Computation*, **2014**, 10, 981-8 | 6.4 | 30 |
| 134 | Chelation-Induced Quenching of Two-Photon Absorption of Azacrown Ether Substituted Distyryl Benzene for Metal Ion Sensing. *Journal of Chemical Theory and Computation*, **2014**, 10, 778-88 | 6.4 | 9 |
| 133 | Lanczos-driven coupled-cluster damped linear response theory for molecules in polarizable environments. *Journal of Chemical Physics*, **2014**, 141, 244107 | 3.9 | 19 |
| 132 | Identifying the Hamiltonian structure in linear response theory. *Journal of Chemical Physics*, **2014**, 140, 224103 | 3.9 | 10 |
| 131 | Low-voltage organic phototransistors based on naphthyl end-capped oligothiophene nanofibers. *Organic Electronics*, **2014**, 15, 1273-1281 | 3.5 | 21 |
| 130 | The Second-Order Polarization Propagator Approximation (SOPPA) method coupled to the polarizable continuum model. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 54-60 | 2 | 8 |
| 129 | Synthesis, biological evaluation and molecular modelling studies of 4-anilinoquinazoline derivatives as protein kinase inhibitors. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 1909-15 | 3.4 | 10 |
| 128 | Inhibitor ranking through QM based chelation calculations for virtual screening of HIV-1 RNase H inhibition. *PLoS ONE*, **2014**, 9, e98659 | 3.7 | 15 |
| 127 | Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. *Molecular Physics*, **2013**, 111, 1235-1248 | 1.7 | 71 |
| 126 | Photoabsorption of acridine yellow and proflavin bound to human serum albumin studied by means of quantum mechanics/molecular dynamics. *Journal of Physical Chemistry B*, **2013**, 117, 2069-80 | 3.4 | 17 |
| 125 | A quantum mechanics/molecular dynamics study of electric field gradient fluctuations in the liquid phase. The case of Na+ in aqueous solution. *Physical Chemistry Chemical Physics*, **2013**, 15, 1621-31 | 3.6 | 12 |
| 124 | On the photophysics of carotenoids: a multireference DFT study of peridinin. *Journal of Physical Chemistry B*, **2013**, 117, 13808-15 | 3.4 | 45 |
| 123 | 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, 4928-38 | 6.4 | 44 |
| 122 | pH-Induced Modulation of One- and Two-Photon Absorption Properties in a Naphthalene-Based Molecular Probe. *Journal of Chemical Theory and Computation*, **2013**, 9, 3660-9 | 6.4 | 10 |
| 121 | A Unified Framework for the Polarizable Embedding and Continuum Methods Within Multiconfigurational Self-consistent Field Theory. *Advances in Quantum Chemistry*, **2013**, 66, 195-238 | 1.4 | 10 |

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| 120 | Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. *Physical Chemistry Chemical Physics*, **2013**, 15, 7567-76 | 3.6 | 25 |
| 119 | EPR spin Hamiltonian parameters of encapsulated spin-labels: impact of the hydrogen bonding topology. *Physical Chemistry Chemical Physics*, **2013**, 15, 2427-34 | 3.6 | 4 |
| 118 | Two-photon solvatochromism II: experimental and theoretical study of solvent effects on the two-photon absorption spectrum of Reichardt© dye. *ChemPhysChem*, **2013**, 14, 3731-9 | 3.2 | 23 |
| 117 | A polarizable embedding DFT study of one-photon absorption in fluorescent proteins. *Physical Chemistry Chemical Physics*, **2013**, 15, 4735-43 | 3.6 | 38 |
| 116 | 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, 2209-20 | 6.4 | 95 |
| 115 | Coordination-driven switching of a preorganized and cooperative calix[4]pyrrole receptor. *Chemistry - A European Journal*, **2013**, 19, 2768-75 | 4.8 | 6 |
| 114 | Energy flow in the cryptophyte PE545 antenna is directed by bilin pigment conformation. *Journal of Physical Chemistry B*, **2013**, 117, 4263-73 | 3.4 | 43 |
| 113 | Validating and Analyzing EPR Hyperfine Coupling Constants with Density Functional Theory. *Journal of Chemical Theory and Computation*, **2013**, 9, 2380-8 | 6.4 | 23 |
| 112 | Association dynamics and linear and nonlinear optical properties of an N-acetylaladanamide probe in a POPC membrane. *Journal of the American Chemical Society*, **2013**, 135, 13590-7 | 16.4 | 24 |
| 111 | Revealing spectral features in two-photon absorption spectrum of Hoechst 33342: a combined experimental and quantum-chemical study. *Journal of Physical Chemistry B*, **2013**, 117, 12013-9 | 3.4 | 18 |
| 110 | Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. *Journal of Physical Chemistry Letters*, **2013**, 4, 70-7 | 6.4 | 26 |
| 109 | The multi-configuration self-consistent field method within a polarizable embedded framework. *Journal of Chemical Physics*, **2013**, 139, 044101 | 3.9 | 40 |
| 108 | Virtual screening models for prediction of HIV-1 RT associated RNase H inhibition. *PLoS ONE*, **2013**, 8, e73478 | 3.7 | 20 |
| 107 | Binding Mechanism and Magnetic Properties of a Multifunctional Spin Label for Targeted EPR Imaging of Amyloid Proteins: Insight from Atomistic Simulations and First-Principles Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 4766-74 | 6.4 | 8 |
| 106 | How Crucial Are Finite Temperature and Solvent Effects on Structure and Absorption Spectra of Si10?. *Journal of Physical Chemistry C*, **2012**, 116, 26618-26624 | 3.8 | 4 |
| 105 | A combined quantum mechanics/molecular mechanics study of the one- and two-photon absorption in the green fluorescent protein. *Physical Chemistry Chemical Physics*, **2012**, 14, 5440-51 | 3.6 | 66 |
| 104 | Color modeling of protein optical probes. *Physical Chemistry Chemical Physics*, **2012**, 14, 1107-12 | 3.6 | 39 |
| 103 | Quantification of the □□ interactions that govern tertiary structure in donor-acceptor [2]pseudorotaxanes. *Journal of the American Chemical Society*, **2012**, 134, 3857-63 | 16.4 | 29 |

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| 102 | Molecular-Level Insight into the Spectral Tuning Mechanism of the DsRed Chromophore. *Journal of Physical Chemistry Letters*, **2012**, 3, 3513-21 | 6.4 | 48 |
| 101 | Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. *Journal of Chemical Theory and Computation*, **2012**, 8, 257-63 | 6.4 | 19 |
| 100 | PERI-CC2: A Polarizable Embedded RI-CC2 Method. *Journal of Chemical Theory and Computation*, **2012**, 8, 3274-83 | 6.4 | 66 |
| 99 | Basis Set Recommendations for DFT Calculations of Gas-Phase Optical Rotation at Different Wavelengths. *Journal of Chemical Theory and Computation*, **2012**, 8, 4425-33 | 6.4 | 22 |
| 98 | NMR spin-spin coupling constants in polymethine dyes as polarity indicators. *Chemistry - A European Journal*, **2012**, 18, 11677-84 | 4.8 | 14 |
| 97 | Parallelization of the polarizable embedding scheme for higher-order response functions. *Molecular Physics*, **2012**, 110, 2579-2586 | 1.7 | 2 |
| 96 | Basis set convergence of indirect spin-spin coupling constants in the Kohn-Sham limit for several small molecules. *Journal of Physical Chemistry A*, **2012**, 116, 3728-38 | 2.8 | 55 |
| 95 | A click chemistry approach to pleuromutilin derivatives, part 2: conjugates with acyclic nucleosides and their ribosomal binding and antibacterial activity. *Journal of Medicinal Chemistry*, **2012**, 55, 2067-77 | 8.3 | 24 |
| 94 | The role of molecular conformation and polarizable embedding for one- and two-photon absorption of disperse orange 3 in solution. *Journal of Physical Chemistry B*, **2012**, 116, 8169-81 | 3.4 | 33 |
| 93 | Performance of popular XC-functionals for the description of excitation energies in GFP-like chromophore models. *International Journal of Quantum Chemistry*, **2012**, 112, 789-800 | 2.1 | 45 |
| 92 | Improving the calculation of Electron Paramagnetic Resonance hyperfine coupling tensors for d-block metals. *Physical Chemistry Chemical Physics*, **2012**, 14, 10669-76 | 3.6 | 27 |
| 91 | On the importance of excited state dynamic response electron correlation in polarizable embedding methods. *Journal of Computational Chemistry*, **2012**, 33, 2012-22 | 3.5 | 33 |
| 90 | Accurate predictions of nonpolar solvation free energies require explicit consideration of binding-site hydration. *Journal of the American Chemical Society*, **2011**, 133, 13081-92 | 16.4 | 53 |
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