# Tomasz A Wesolowski

List of Publications by Year
in descending order



| 83 | 5,518 | 126907 | 79698 |
|---|---|---|---|
| papers | citations | 33 h-index | 73 g-index |

| 89 | 89 | 89 | 3240 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | A non-decomposable approximation on the complete density function space for the non-additive kinetic potential. Journal of Chemical Physics, 2022, 156, 044103. | 3.0 | 4 |
| 2 | Quantifying Fluctuations of Average Solvent Environments for Embedding Calculations. Journal of Chemical Theory and Computation, 2022, 18, 1072-1088. | 5.3 | 4 |
| 3 | N-representability of the target density in Frozen-Density Embedding Theory based methods: Numerical significance and its relation to electronic polarization. Journal of Chemical Physics, 2022, 157, . | 3.0 | 4 |
| 4 | Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269. | 2.5 | 26 |
| 5 | The Challenge of Accurate Computation of Two-Photon Absorption Properties of Organic Chromophores in the Condensed Phase. Journal of Chemical Theory and Computation, 2021, 17, 3652-3665. | 5.3 | 5 |
| 6 | Benchmark of the Extension of Frozen-Density Embedding Theory to Nonvariational Correlated Methods: The Embedded-MP2 Case. Journal of Chemical Theory and Computation, 2021, 17, 4049-4062. | 5.3 | 4 |
| 7 | Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801. | 3.0 | 518 |
| 8 | On the Correlation Potential in Frozen-Density Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 6880-6885. | 5.3 | 15 |
| 9 | Embedding-theory-based simulations using experimental electron densities for the environment. Acta Crystallographica Section A: Foundations and Advances, 2020, 76, 571-579. | 0.1 | 7 |
| 10 | OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964. | 5.3 | 661 |
| 11 | The deconvolution analysis of ATR-FTIR spectra of diacetylene during UV exposure. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 219, 23-32. | 3.9 | 12 |
| 12 | Origin of the Solvatochromism in Organic Fluorophores with Flexible Side Chains: A Case Study of Flugi-2. Journal of Physical Chemistry A, 2019, 123, 4581-4587. | 2.5 | 3 |
| 13 | Extension of frozen-density embedding theory for non-variational embedded wavefunctions. Journal of Chemical Physics, 2019, 150, 121101. | 3.0 | 9 |
| 14 | Size extensivity of elastic properties of alkane fragments. Journal of Molecular Modeling, 2018, 24, 36. | 1.8 | 4 |
| 15 | Nonadditive kinetic potentials from inverted Kohnâ€“Sham problem. International Journal of Quantum Chemistry, 2018, 118, e25410. | 2.0 | 16 |
| 16 | Explicit vs. implicit electronic polarisation of environment of an embedded chromophore in frozen-density embedding theory. Physical Chemistry Chemical Physics, 2018, 20, 26053-26062. | 2.8 | 12 |
| 17 | Benchmark of Excitation Energy Shifts from Frozen-Density Embedding Theory: Introduction of a Density-Overlap-Based Applicability Threshold. Journal of Chemical Theory and Computation, 2018, 14, 4028-4040. | 5.3 | 16 |
| 18 | Implementation and Application of the Frozen Density Embedding Theory with the Algebraic Diagrammatic Construction Scheme for the Polarization Propagator up to Third Order. Journal of Chemical Theory and Computation, 2017, 13, 4711-4725. | 5.3 | 21 |

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|---|---|---|---|
| 19 | First time combination of frozen density embedding theory with the algebraic diagrammatic construction scheme for the polarization propagator of second order. Journal of Chemical Physics, 2016, 144, 204103. | 3.0 | 30 |
| 20 | Frozen-density embedding theory with average solvent charge densities from explicit atomistic simulations. Physical Chemistry Chemical Physics, 2016, 18, 21069-21078. | 2.8 | 13 |
| 21 | Fluorescence quantum yield rationalized by the magnitude of the charge transfer in Ï€-conjugated terpyridine derivatives. Physical Chemistry Chemical Physics, 2016, 18, 29387-29394. | 2.8 | 21 |
| 22 | Looking for the Origin of Allosteric Cooperativity in Metallopolymers. Chemistry - A European Journal, 2016, 22, 8113-8123. | 3.3 | 21 |
| 23 | Homogeneity properties of the embedding potential in frozen-density embedding theory. Molecular Physics, 2016, 114, 1199-1206. | 1.7 | 5 |
| 24 | Orthogonality of embedded wave functions for different states in frozen-density embedding theory. Journal of Chemical Physics, 2015, 143, 164106. | 3.0 | 19 |
| 25 | Frozen-Density Embedding Strategy for Multilevel Simulations of Electronic Structure. Chemical Reviews, 2015, 115, 5891-5928. | 47.7 | 258 |
| 26 | Nonuniform Continuum Model for Solvatochromism Based on Frozenâ€Density Embedding Theory. ChemPhysChem, 2014, 15, 3291-3300. | 2.1 | 10 |
| 27 | Embedding potentials for excited states of embedded species. Journal of Chemical Physics, 2014, 140, 18A530. | 3.0 | 27 |
| 28 | How to choose the frozen density in Frozen-Density Embedding Theory-based numerical simulations of local excitations?. Theoretical Chemistry Accounts, 2014, 133, 1. | 1.4 | 39 |
| 29 | Spectral Tuning of Rhodopsin and Visual Cone Pigments. Journal of the American Chemical Society, 2014, 136, 2723-2726. | 13.7 | 43 |
| 30 | Non-uniform Continuum Model for Solvated Species Based on Frozen-Density Embedding Theory: The Study Case of Solvatochromism of Coumarin 153. Chimia, 2014, 68, 609. | 0.6 | 3 |
| 31 | First-principles simulation of the absorption bands of fluorenone in zeolite L. Physical Chemistry Chemical Physics, 2013, 15, 159-167. | 2.8 | 38 |
| 32 | Non-Additive Kinetic Energy and Potential in Analytically Solvable Systems and Their Approximated Counterparts. Recent Advances in Computational, 2013, , 275-295. | 0.8 | 12 |
| 33 | Semilocal Approximations for the Kinetic Energy. Recent Advances in Computational, 2013, , 429-442. | 0.8 | 17 |
| 34 | Exact non-additive kinetic potentials in realistic chemical systems. Journal of Chemical Physics, 2012, 137, 094110. | 3.0 | 27 |
| 35 | Pure-state noninteracting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>v</mml:mi></mml:math>-representability of electron densities from Kohn-Sham calculations with finite basis sets. Physical Review A, 2012, 85, . | 2.5 | 24 |
| 36 | Importance of the Intermolecular Pauli Repulsion in Embedding Calculations for Molecular Properties: The Case of Excitation Energies for a Chromophore in Hydrogen-Bonded Environments. Journal of Physical Chemistry A, 2011, 115, 10018-10026. | 2.5 | 33 |

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| 37 | The Importance of Going beyond Coulombic Potential in Embedding Calculations for Molecular Properties: The Case of Iso-G for Biliverdin in Protein-Like Environment. Journal of Chemical Theory and Computation, 2011, 7, 213-222. | 5.3 | 24 |
| 38 | Embedding vs Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excitation Energies. Journal of Chemical Theory and Computation, 2011, 7, 1647-1666. | 5.3 | 63 |
| 39 | Multi-scale modelling of solvatochromic shifts from frozen-density embedding theory with non-uniform continuum model of the solvent: the coumarin 153 case. Physical Chemistry Chemical Physics, 2011, 13, 10565. | 2.8 | 30 |
| 40 | Self-consistency in frozen-density embedding theory based calculations. Journal of Chemical Physics, 2011, 135, 084120. | 3.0 | 23 |
| 41 | Modeling Solvatochromic Shifts Using the Orbital-Free Embedding Potential at Statistically Mechanically Averaged Solvent Density. Journal of Physical Chemistry A, 2010, 114, 6082-6096. | 2.5 | 84 |
| 42 | Linearized orbitalâ€free embedding potential in selfâ€consistent calculations. International Journal of Quantum Chemistry, 2009, 109, 1886-1897. | 2.0 | 14 |
| 43 | Orbitalâ€free effective embedding potential: Densityâ€matrix functional theory case. International Journal of Quantum Chemistry, 2009, 109, 2520-2525. | 2.0 | 46 |
| 44 | Cooperative Effect of Hydrogen-Bonded Chains in the Environment of a Ï€ â†’ Ï€* Chromophore. Journal of Physical Chemistry A, 2009, 113, 9766-9771. | 2.5 | 18 |
| 45 | Orbital-Free Embedding Effective Potential in Analytically Solvable Cases. Progress in Theoretical Chemistry and Physics, 2009, , 311-326. | 0.2 | 13 |
| 46 | Embedding a multideterminantal wave function in an orbital-free environment. Physical Review A, 2008, 77, . | 2.5 | 138 |
| 47 | Orbital-free effective embedding potential at nuclear cusps. Journal of Chemical Physics, 2008, 129, 074107. | 3.0 | 50 |
| 48 | The energy-differences based exact criterion for testing approximations to the functional for the kinetic energy of non-interacting electrons. Journal of Physics A: Mathematical and Theoretical, 2008, 41, 055302. | 2.1 | 33 |
| 49 | Equilibrium Geometries of Noncovalently Bound Intermolecular Complexes Derived from Subsystem Formulation of Density Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 735-745. | 5.3 | 45 |
| 50 | Interaction energies in non-covalently bound intermolecular complexes derived using the subsystem formulation of density functional theory. Journal of Molecular Modeling, 2007, 13, 631-642. | 1.8 | 26 |
| 51 | On the electron leak problem in orbital-free embedding calculations. Journal of Chemical Physics, 2006, 124, 164101. | 3.0 | 35 |
| 52 | One-Electron Equations for Embedded Electron Density: Challenge for Theory and Practical Payoffs in Multi-Level Modelling of Complex Polyatomic Systems. Computational Chemistry - Reviews of Current Trends, 2006, , 1-82. | 0.4 | 88 |
| 53 | The basis set effect on the results of the minimization of the total energy bifunctionalE[?A,?B]. International Journal of Quantum Chemistry, 2005, 101, 543-549. | 2.0 | 24 |
| 54 | Theoretical study of neutral and cationic complexes involving phenol. International Journal of Quantum Chemistry, 2005, 101, 854-859. | 2.0 | 9 |

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| 55 | The merits of the frozen-density embedding scheme to model solvatochromic shifts. Journal of Chemical Physics, 2005, 122, 094115. | 3.0 | 207 |
| 56 | Approximating the kinetic energy functionalT<sub>s</sub>[ï¿½: lessons from four-electron systems. Molecular Physics, 2005, 103, 1165-1167. | 1.7 | 11 |
| 57 | An Explicit Quantum Chemical Method for Modeling Large Solvation Shells Applied to Aminocoumarin C151. Journal of Physical Chemistry A, 2005, 109, 7805-7814. | 2.5 | 130 |
| 58 | Modeling solvent effects on electron-spin-resonance hyperfine couplings by frozen-density embedding. Journal of Chemical Physics, 2005, 123, 114101. | 3.0 | 64 |
| 59 | One-Electron Equations for Embedded Electron Density and Their Applications to Study Electronic Structure of Atoms and Molecules in Condensed Phase. Chimia, 2005, 59, 488-492. | 0.6 | 2 |
| 60 | Generalization of the Kohn-Sham equations with constrained electron density formalism and its time-dependent response theory formulation. International Journal of Quantum Chemistry, 2004, 96, 577-588. | 2.0 | 178 |
| 61 | Application of the density functional theory derived orbital-free embedding potential to calculate the splitting energies of lanthanide cations in chloroelpasolite crystals. Chemical Physics Letters, 2004, 397, 441-446. | 2.6 | 52 |
| 62 | Theoretical Investigation of the Anion Binding Affinities of the Uranyl Salophene Complexes. Journal of Physical Chemistry A, 2004, 108, 5091-5099. | 2.5 | 19 |
| 63 | Hydrogen-Bonding-Induced Shifts of the Excitation Energies in Nucleic Acid Bases:â€‰ An Interplay between Electrostatic and Electron Density Overlap Effects. Journal of the American Chemical Society, 2004, 126, 11444-11445. | 13.7 | 127 |
| 64 | Ï€-Stacking Behavior of Selected Nitrogen-Containing PAHs. Journal of Physical Chemistry A, 2004, 108, 9155-9160. | 2.5 | 17 |
| 65 | Quantum Chemistry 'Without Orbitals' â€“ An Old Idea and Recent Developments. Chimia, 2004, 58, 311-315. | 0.6 | 23 |
| 66 | A Highly Configurationally Stable [4]Heterohelicenium Cation. Angewandte Chemie - International Edition, 2003, 42, 3162-3166. | 13.8 | 124 |
| 67 | Gradient-free and gradient-dependent approximations in the total energy bifunctional for weakly overlapping electron densities. Journal of Chemical Physics, 2003, 118, 2072-2080. | 3.0 | 77 |
| 68 | Density Functional Study of a Helical Organic Cation. Chimia, 2003, 57, 173-174. | 0.6 | 3 |
| 69 | Comment on â€œPrediction of Electronic Excited States of Adsorbates on Metal Surfaces from First Principlesâ€• Physical Review Letters, 2002, 88, 209701; author reply 209702. | 7.8 | 14 |
| 70 | Development of Novel Computational Strategies to Match the Challenges of Supramolecular Chemistry, Biochemistry, and Materials Science. Chimia, 2002, 56, 707-711. | 0.6 | 3 |
| 71 | Physisorption of Molecular Hydrogen on Polycyclic Aromatic Hydrocarbons:â€‰ A Theoretical Study. Journal of Physical Chemistry B, 2002, 106, 8689-8696. | 2.6 | 54 |
| 72 | Link between the kinetic- and exchange-energy functionals in the generalized gradient approximation. International Journal of Quantum Chemistry, 2002, 89, 441-446. | 2.0 | 97 |

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| 73 | Introduction of the explicit long-range nonlocality as an alternative to the gradient expansion approximation for the kinetic-energy functional. Chemical Physics Letters, 2002, 360, 209-216. | 2.6 | 9 |
| 74 | Constraining the electron densities in DFT method as an effective way forab initio studies of metal-catalyzed reactions. Journal of Computational Chemistry, 2000, 21, 1554-1561. | 3.3 | 44 |
| 75 | Theoretical Study of the Physisorption of CO on Metal Oxide Surfaces Using the KSCED-DFT Approach. Collection of Czechoslovak Chemical Communications, 1998, 63, 1447-1459. | 1.0 | 5 |
| 76 | Density functional theory with approximate kinetic energy functionals applied to hydrogen bonds. Journal of Chemical Physics, 1997, 106, 8516-8526. | 3.0 | 139 |
| 77 | Kohn-Sham equations with constrained electron density: The effect of various kinetic energy functional parametrizations on the ground-state molecular properties. International Journal of Quantum Chemistry, 1997, 61, 303-311. | 2.0 | 50 |
| 78 | Kohnâ€Sham equations with constrained electron density: The effect of various kinetic energy functional parametrizations on the groundâ€state molecular properties. International Journal of Quantum Chemistry, 1997, 61, 303-311. | 2.0 | 8 |
| 79 | Kohn-Sham equations with constrained electron density: an iterative evaluation of the ground-state electron density of interacting molecules. Chemical Physics Letters, 1996, 248, 71-76. | 2.6 | 241 |
| 80 | Accuracy of approximate kinetic energy functionals in the model of Kohnâ€“Sham equations with constrained electron density: The FHâ‹…â‹…â‹…NCH complex as a test case. Journal of Chemical Physics, 1996, 105, 9182-9190. | 3.0 | 123 |
| 81 | Ab Initio Frozen Density Functional Calculations of Proton Transfer Reactions in Solution. The Journal of Physical Chemistry, 1996, 100, 15444-15449. | 2.9 | 112 |
| 82 | Frozen density functional approach for ab initio calculations of solvated molecules. The Journal of Physical Chemistry, 1993, 97, 8050-8053. | 2.9 | 701 |
| 83 | Quantumâ€mechanical calculations of solvation free energies. A combinedabinitiopseudopotential freeâ€energy perturbation approach. Journal of Chemical Physics, 1992, 97, 4264-4271. | 3.0 | 68 |