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	Frozen density functional approach for ab initio calculations of solvated molecules. The Journal of Physical Chemistry, 1993, 97, 8050-8053.	2.9	701
2	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
3	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
4	Frozen-Density Embedding Strategy for Multilevel Simulations of Electronic Structure. Chemical Reviews, 2015, 115, 5891-5928.	47.7	258
5	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
6	The merits of the frozen-density embedding scheme to model solvatochromic shifts. Journal of Chemical Physics, 2005, 122, 094115.	3.0	207
7	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
8	Density functional theory with approximate kinetic energy functionals applied to hydrogen bonds. Journal of Chemical Physics, 1997, 106, 8516-8526.	3.0	139
9	Embedding a multideterminantal wave function in an orbital-free environment. Physical Review A, 2008, 77, .	2.5	138
10	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
11	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
12	A Highly Configurationally Stable [4]Heterohelicenium Cation. Angewandte Chemie - International Edition, 2003, 42, 3162-3166.	13.8	124
13	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
14	Ab Initio Frozen Density Functional Calculations of Proton Transfer Reactions in Solution. The Journal of Physical Chemistry, 1996, 100, 15444-15449.	2.9	112
15	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
16	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
17	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
18	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

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19	Quantumâ€mechanical calculations of solvation free energies. A combinedabinitiopseudopotential freeâ€energy perturbation approach. Journal of Chemical Physics, 1992, 97, 4264-4271.	3.0	68
20	Modeling solvent effects on electron-spin-resonance hyperfine couplings by frozen-density embedding. Journal of Chemical Physics, 2005, 123, 114101.	3.0	64
21	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
22	Physisorption of Molecular Hydrogen on Polycyclic Aromatic Hydrocarbons:â€‰ A Theoretical Study. Journal of Physical Chemistry B, 2002, 106, 8689-8696.	2.6	54
23	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
24	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
25	Orbital-free effective embedding potential at nuclear cusps. Journal of Chemical Physics, 2008, 129, 074107.	3.0	50
26	Orbitalâ€free effective embedding potential: Densityâ€matrix functional theory case. International Journal of Quantum Chemistry, 2009, 109, 2520-2525.	2.0	46
27	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
28	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
29	Spectral Tuning of Rhodopsin and Visual Cone Pigments. Journal of the American Chemical Society, 2014, 136, 2723-2726.	13.7	43
30	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
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	On the electron leak problem in orbital-free embedding calculations. Journal of Chemical Physics, 2006, 124, 164101.	3.0	35
33	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
34	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
35	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
36	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

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37	Exact non-additive kinetic potentials in realistic chemical systems. Journal of Chemical Physics, 2012, 137, 094110.	3.0	27
38	Embedding potentials for excited states of embedded species. Journal of Chemical Physics, 2014, 140, 18A530.	3.0	27
39	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
40	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	2.5	26
41	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
42	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
43	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
44	Quantum Chemistry 'Without Orbitals' â€“ An Old Idea and Recent Developments. Chimia, 2004, 58, 311-315.	0.6	23
45	Self-consistency in frozen-density embedding theory based calculations. Journal of Chemical Physics, 2011, 135, 084120.	3.0	23
46	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
47	Looking for the Origin of Allosteric Cooperativity in Metallopolymers. Chemistry - A European Journal, 2016, 22, 8113-8123.	3.3	21
48	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
49	Theoretical Investigation of the Anion Binding Affinities of the Uranyl Salophene Complexes. Journal of Physical Chemistry A, 2004, 108, 5091-5099.	2.5	19
50	Orthogonality of embedded wave functions for different states in frozen-density embedding theory. Journal of Chemical Physics, 2015, 143, 164106.	3.0	19
51	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
52	Ï€-Stacking Behavior of Selected Nitrogen-Containing PAHs. Journal of Physical Chemistry A, 2004, 108, 9155-9160.	2.5	17
53	Semilocal Approximations for the Kinetic Energy. Recent Advances in Computational, 2013, , 429-442.	0.8	17
54	Nonadditive kinetic potentials from inverted Kohnâ€“Sham problem. International Journal of Quantum Chemistry, 2018, 118, e25410.	2.0	16

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55	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
56	On the Correlation Potential in Frozen-Density Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 6880-6885.	5.3	15
57	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
58	Linearized orbitalâ€free embedding potential in selfâ€consistent calculations. International Journal of Quantum Chemistry, 2009, 109, 1886-1897.	2.0	14
59	Frozen-density embedding theory with average solvent charge densities from explicit atomistic simulations. Physical Chemistry Chemical Physics, 2016, 18, 21069-21078.	2.8	13
60	Orbital-Free Embedding Effective Potential in Analytically Solvable Cases. Progress in Theoretical Chemistry and Physics, 2009, , 311-326.	0.2	13
61	Non-Additive Kinetic Energy and Potential in Analytically Solvable Systems and Their Approximated Counterparts. Recent Advances in Computational, 2013, , 275-295.	0.8	12
62	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
63	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
64	Approximating the kinetic energy functionalT_s[ï¿½]: lessons from four-electron systems. Molecular Physics, 2005, 103, 1165-1167.	1.7	11
65	Nonuniform Continuum Model for Solvatochromism Based on Frozenâ€Density Embedding Theory. ChemPhysChem, 2014, 15, 3291-3300.	2.1	10
66	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
67	Theoretical study of neutral and cationic complexes involving phenol. International Journal of Quantum Chemistry, 2005, 101, 854-859.	2.0	9
68	Extension of frozen-density embedding theory for non-variational embedded wavefunctions. Journal of Chemical Physics, 2019, 150, 121101.	3.0	9
69	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
70	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
71	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
72	Homogeneity properties of the embedding potential in frozen-density embedding theory. Molecular Physics, 2016, 114, 1199-1206.	1.7	5

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73	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
74	Size extensivity of elastic properties of alkane fragments. Journal of Molecular Modeling, 2018, 24, 36.	1.8	4
75	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
76	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
77	Quantifying Fluctuations of Average Solvent Environments for Embedding Calculations. Journal of Chemical Theory and Computation, 2022, 18, 1072-1088.	5.3	4
78	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
79	Development of Novel Computational Strategies to Match the Challenges of Supramolecular Chemistry, Biochemistry, and Materials Science. Chimia, 2002, 56, 707-711.	0.6	3
80	Density Functional Study of a Helical Organic Cation. Chimia, 2003, 57, 173-174.	0.6	3
81	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
82	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
83	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