

Aleksandr V Marenich

List of Publications by Year in descending order

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Version: 2024-02-01

22
papers

18,577
citations

361045

20
h-index

642321

23
g-index

23
all docs

23
docs citations

23
times ranked

19962
citing authors

#	ARTICLE	IF	CITATIONS
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
2	Electronic Absorption Spectra and Solvatochromic Shifts by the Vertical Excitation Model: Solvated Clusters and Molecular Dynamics Sampling. <i>Journal of Physical Chemistry B</i> , 2015, 119, 958-967.	1.2	68
3	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
4	Configuration Interaction-Corrected Tamm-Dancoff Approximation: A Time-Dependent Density Functional Method with the Correct Dimensionality of Conical Intersections. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 322-328.	2.1	45
5	Computational electrochemistry: prediction of liquid-phase reduction potentials. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 15068-15106.	1.3	407
6	Uniform Treatment of Solute Solvent Dispersion in the Ground and Excited Electronic States of the Solute Based on a Solvation Model with State-Specific Polarizability. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3649-3659.	2.3	59
7	Generalized Born Solvation Model SM12. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 609-620.	2.3	170
8	Reduced and quenched polarizabilities of interior atoms in molecules. <i>Chemical Science</i> , 2013, 4, 2349.	3.7	56
9	Construction of Pourbaix Diagrams for Ruthenium-Based Water Oxidation Catalysts by Density Functional Theory. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 12810-12814.	7.2	54
10	Resolution of a Challenge for Solvation Modeling: Calculation of Dicarboxylic Acid Dissociation Constants Using Mixed Discrete-Continuum Solvation Models. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1437-1442.	2.1	76
11	Charge Model 5: An Extension of Hirshfeld Population Analysis for the Accurate Description of Molecular Interactions in Gaseous and Condensed Phases. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 527-541.	2.3	661
12	Practical computation of electronic excitation in solution: vertical excitation model. <i>Chemical Science</i> , 2011, 2, 2143.	3.7	202
13	Sorting Out the Relative Contributions of Electrostatic Polarization, Dispersion, and Hydrogen Bonding to Solvatochromic Shifts on Vertical Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2829-2844.	2.3	45
14	Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. <i>Journal of Physical Chemistry B</i> , 2009, 113, 6378-6396.	1.2	12,475
15	Solvent Dependence of ^{14}N Nuclear Magnetic Resonance Chemical Shielding Constants as a Test of the Accuracy of the Computed Polarization of Solute Electron Densities by the Solvent. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2284-2300.	2.3	9
16	Mechanistic Analysis of the Base-Catalyzed HF Elimination from 4-Fluoro-4-(4-nitrophenyl)butane-2-one Based on Liquid-Phase Kinetic Isotope Effects Calculated by Dynamics Modeling with Multidimensional Tunneling. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 59-67.	2.3	8
17	Universal Solvation Model Based on the Generalized Born Approximation with Asymmetric Descreening. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2447-2464.	2.3	120
18	Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-Molecule Solvation Free Energies. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4538-4543.	1.2	418

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19	Perspective on Foundations of Solvation Modeling: The Electrostatic Contribution to the Free Energy of Solvation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 877-887.	2.3	62
20	Self-Consistent Reaction Field Model for Aqueous and Nonaqueous Solutions Based on Accurate Polarized Partial Charges. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2011-2033.	2.3	426
21	Charge Model 4 and Intramolecular Charge Polarization. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2046-2054.	2.3	75
22	Polarization Effects in Aqueous and Nonaqueous Solutions. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2055-2067.	2.3	55