Aleksandr V Marenich

List of Publications by Year
in descending order

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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	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. Journal of Physical Chemistry B, 2009, 113, 6378-6396.	1.2	12,475
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Charge Model 5: An Extension of Hirshfeld Population Analysis for the Accurate Description of Molecular Interactions in Gaseous and Condensed Phases. Journal of Chemical Theory and Computation, 2012, 8, 527-541.	2.3	661
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
5	Self-Consistent Reaction Field Model for Aqueous and Nonaqueous Solutions Based on Accurate Polarized Partial Charges. Journal of Chemical Theory and Computation, 2007, 3, 2011-2033.	2.3	426
6	Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-Molecule Solvation Free Energies. Journal of Physical Chemistry B, 2009, 113, 4538-4543.	1.2	418
7	Computational electrochemistry: prediction of liquid-phase reduction potentials. Physical Chemistry Chemical Physics, 2014, 16, 15068-15106.	1.3	407
8	Practical computation of electronic excitation in solution: vertical excitation model. Chemical Science, 2011, 2, 2143.	3.7	202
9	Generalized Born Solvation Model SM12. Journal of Chemical Theory and Computation, 2013, 9, 609-620.	2.3	170
10	Universal Solvation Model Based on the Generalized Born Approximation with Asymmetric Descreening. Journal of Chemical Theory and Computation, 2009, 5, 2447-2464.	2.3	120
11	Resolution of a Challenge for Solvation Modeling: Calculation of Dicarboxylic Acid Dissociation Constants Using Mixed Discreteâ€“Continuum Solvation Models. Journal of Physical Chemistry Letters, 2012, 3, 1437-1442.	2.1	76
12	Charge Model 4 and Intramolecular Charge Polarization. Journal of Chemical Theory and Computation, 2007, 3, 2046-2054.	2.3	75
13	Electronic Absorption Spectra and Solvatochromic Shifts by the Vertical Excitation Model: Solvated Clusters and Molecular Dynamics Sampling. Journal of Physical Chemistry B, 2015, 119, 958-967.	1.2	68
14	Perspective on Foundations of Solvation Modeling: The Electrostatic Contribution to the Free Energy of Solvation. Journal of Chemical Theory and Computation, 2008, 4, 877-887.	2.3	62
15	Uniform Treatment of Soluteâ€“Solvent Dispersion in the Ground and Excited Electronic States of the Solute Based on a Solvation Model with State-Specific Polarizability. Journal of Chemical Theory and Computation, 2013, 9, 3649-3659.	2.3	59
16	Reduced and quenched polarizabilities of interior atoms in molecules. Chemical Science, 2013, 4, 2349.	3.7	56
17	Polarization Effects in Aqueous and Nonaqueous Solutions. Journal of Chemical Theory and Computation, 2007, 3, 2055-2067.	2.3	55
18	Construction of Pourbaix Diagrams for Rutheniumâ€Based Waterâ€Oxidation Catalysts by Density Functional Theory. Angewandte Chemie - International Edition, 2012, 51, 12810-12814.	7.2	54

#	Article	IF	Citations
19	Sorting Out the Relative Contributions of Electrostatic Polarization, Dispersion, and Hydrogen Bonding to Solvatochromic Shifts on Vertical Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2010, 6, 2829-2844.	2.3	45
20	Configuration Interaction-Corrected Tammâ€“Dancoff Approximation: A Time-Dependent Density Functional Method with the Correct Dimensionality of Conical Intersections. Journal of Physical Chemistry Letters, 2014, 5, 322-328.	2.1	45
21	Solvent Dependence of¹⁴N Nuclear Magnetic Resonance Chemical Shielding Constants as a Test of the Accuracy of the Computed Polarization of Solute Electron Densities by the Solvent. Journal of Chemical Theory and Computation, 2009, 5, 2284-2300.	2.3	9
22	Mechanistic Analysis of the Base-Catalyzed HF Elimination from 4-Fluoro-4-(4â€²-nitrophenyl)butane-2-one Based on Liquid-Phase Kinetic Isotope Effects Calculated by Dynamics Modeling with Multidimensional Tunneling. Journal of Chemical Theory and Computation, 2009, 5, 59-67.	2.3	8