Aleksandr V Marenich

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	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.	2.6	68
3	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
4	Configuration Interaction-Corrected Tamm–Dancoff Approximation: A Time-Dependent Density Functional Method with the Correct Dimensionality of Conical Intersections. Journal of Physical Chemistry Letters, 2014, 5, 322-328.	4.6	45
5	Computational electrochemistry: prediction of liquid-phase reduction potentials. Physical Chemistry Chemical Physics, 2014, 16, 15068-15106.	2.8	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. Journal of Chemical Theory and Computation, 2013, 9, 3649-3659.	5.3	59
7	Generalized Born Solvation Model SM12. Journal of Chemical Theory and Computation, 2013, 9, 609-620.	5.3	170
8	Reduced and quenched polarizabilities of interior atoms in molecules. Chemical Science, 2013, 4, 2349.	7.4	56
9	Construction of Pourbaix Diagrams for Rutheniumâ€Based Waterâ€Oxidation Catalysts by Density Functional Theory. Angewandte Chemie - International Edition, 2012, 51, 12810-12814.	13.8	54
10	Resolution of a Challenge for Solvation Modeling: Calculation of Dicarboxylic Acid Dissociation Constants Using Mixed Discrete–Continuum Solvation Models. Journal of Physical Chemistry Letters, 2012, 3, 1437-1442.	4.6	76
11	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.	5.3	661
12	Practical computation of electronic excitation in solution: vertical excitation model. Chemical Science, 2011, 2, 2143.	7.4	202
13	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.	5.3	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. Journal of Physical Chemistry B, 2009, 113, 6378-6396.	2.6	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. Journal of Chemical Theory and Computation, 2009, 5, 2284-2300.	5.3	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. Journal of Chemical Theory and Computation, 2009, 5, 59-67.	5.3	8
17	Universal Solvation Model Based on the Generalized Born Approximation with Asymmetric Descreening. Journal of Chemical Theory and Computation, 2009, 5, 2447-2464.	5.3	120
18	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.	2.6	418

#	Article	IF	CITATIONS
19	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.	5.3	62
20	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.	5.3	426
21	Charge Model 4 and Intramolecular Charge Polarization. Journal of Chemical Theory and Computation, 2007, 3, 2046-2054.	5.3	75
22	Polarization Effects in Aqueous and Nonaqueous Solutions. Journal of Chemical Theory and Computation, 2007, 3, 2055-2067.	5.3	55