Marat Valiev

List of Publications by Year
in descending order

57 papers	6,773 citations	279798 23 h-index	149698 56 g-index
59 all docs	59 docs citations	59 times ranked	11043 citing authors

#	Article	IF	Citations
1	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	7.5	4,740
2	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
3	Fast electron correlation methods for molecular clusters in the ground and excited states. Molecular Physics, 2005, 103, 2255-2265.	1.7	137
4	On the Electronically Excited States of Uracil. Journal of Physical Chemistry A, 2008, 112, 9983-9992.	2.5	115
5	The Role of the Putative Catalytic Base in the Phosphoryl Transfer Reaction in a Protein Kinase:Â First-Principles Calculations. Journal of the American Chemical Society, 2003, 125, 9926-9927.	13.7	108
6	Phosphorylation Reaction in cAPK Protein Kinase-Free Energy Quantum Mechanical/Molecular Mechanics Simulations. Journal of Physical Chemistry B, 2007, 111, 13455-13464.	2.6	106
7	Hybrid approach for free energy calculations with high-level methods: Application to the SN2 reaction of CHCl3 and OHâ^' in water. Journal of Chemical Physics, 2007, 127, 051102.	3.0	70
8	Vertical Ionization Potentials of Nucleobases in a Fully Solvated DNA Environment. Journal of Physical Chemistry B, 2010, 114, 5886-5894.	2.6	69
9	Excitation Energies of Zinc Porphyrin in Aqueous Solution Using Long-Range Corrected Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 6041-6043.	2.5	60
10	Simulating Ru L₃-Edge X-ray Absorption Spectroscopy with Time-Dependent Density Functional Theory: Model Complexes and Electron Localization in Mixed-Valence Metal Dimers. Journal of Physical Chemistry A, 2013, 117, 4444-4454.	2.5	59
11	Hybrid coupled cluster and molecular dynamics approach: Application to the excitation spectrum of cytosine in the native DNA environment. Journal of Chemical Physics, 2006, 125, 211101.	3.0	51
12	Large-scale parallel calculations with combined coupled cluster and molecular mechanics formalism: Excitation energies of zincâ€“porphyrin in aqueous solution. Chemical Physics Letters, 2008, 458, 205-209.	2.6	46
13	Hybrid Quantum Mechanical/Molecular Mechanics Study of the S_N2 Reaction of CH₃Cl+OH^{â€“} in Water. Journal of Physical Chemistry A, 2011, 115, 12047-12052.	2.5	41
14	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
15	Calculations of the electronic structure of 3d transition metal dimers with projector augmented plane wave method. Journal of Chemical Physics, 2003, 119, 5955-5964.	3.0	36
16	Combined Quantum Mechanical and Molecular Mechanics Studies of the Electron-Transfer Reactions Involving Carbon Tetrachloride in Solution. Journal of Physical Chemistry A, 2008, 112, 2713-2720.	2.5	36
17	Parallel implementation of the projector augmented plane wave method for charged systems. Computer Physics Communications, 2002, 143, 11-28.	7.5	35
18	A Dianionic Phosphorane Intermediate and Transition States in an Associative A_N+D_N Mechanism for the RibonucleaseA Hydrolysis Reaction. Journal of the American Chemical Society, 2009, 131, 3869-3871.	13.7	32

#	Article	IF	Citations
19	Integral Equation Theory of Molecular Solvation Coupled with Quantum Mechanical/Molecular Mechanics Method in NWChem Package. Journal of Chemical Theory and Computation, 2012, 8, 1246-1254.	5.3	31
20	The Projector-Augmented Plane Wave Method Applied to Molecular Bonding. Journal of Physical Chemistry A, 1999, 103, 10588-10601.	2.5	27
21	NWChem: scalable parallel computational chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 888-894.	14.6	27
22	Hybrid Quantum Mechanical and Molecular Mechanics Study of the S_N2 Reaction of CCl₄ + OH^{â€“} in Aqueous Solution: The Potential of Mean Force, Reaction Energetics, and Rate Constants. Journal of Physical Chemistry A, 2012, 116, 2371-2376.	2.5	26
23	Study of Ion Specific Interactions of Alkali Cations with Dicarboxylate Dianions. Journal of Physical Chemistry A, 2012, 116, 2055-2061.	2.5	24
24	Density-functional theory of one-electron propagators. Physics Letters, Section A: General, Atomic and Solid State Physics, 1997, 227, 265-270.	2.1	23
25	Asymptotic Extrapolation Scheme for Large-Scale Calculations with Hybrid Coupled Cluster and Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2006, 110, 13106-13111.	2.5	22
26	Communication: Solute anisotropy effects in hydrated anion and neutral clusters. Journal of Chemical Physics, 2013, 138, 031101.	3.0	22
27	Formation of (HCOO^{â€“})(H₂SO₄) Anion Clusters: Violation of Gas-Phase Acidity Predictions. Journal of the American Chemical Society, 2017, 139, 11321-11324.	13.7	22
28	How Anion Chaotrope Changes the Local Structure of Water: Insights from Photoelectron Spectroscopy and Theoretical Modeling of SCN^{â€“} Water Clusters. Journal of Physical Chemistry B, 2016, 120, 1518-1525.	2.6	20
29	Probing microhydration effect on the electronic structure of the GFP chromophore anion: Photoelectron spectroscopy and theoretical investigations. Journal of Chemical Physics, 2015, 143, 224301.	3.0	18
30	Structures and energetics of hydrated deprotonated cis-pinonic acid anion clusters and their atmospheric relevance. Physical Chemistry Chemical Physics, 2017, 19, 10676-10684.	2.8	17
31	Extensive regularization of the coupled cluster methods based on the generating functional formalism: Application to gas-phase benchmarks and to the SN2 reaction of CHCl3 and OHâ^' in water. Journal of Chemical Physics, 2009, 131, 234107.	3.0	15
32	Cryogenic â€œIodide-Taggingâ€•Photoelectron Spectroscopy: A Sensitive Probe for Specific Binding Sites of Amino Acids. Journal of Physical Chemistry Letters, 2020, 11, 4346-4352.	4.6	15
33	Application of High-Level Iterative Coupled-Cluster Methods to the Cytosine Molecule. Journal of Physical Chemistry A, 2008, 112, 5538-5541.	2.5	14
34	Deprotonated Dicarboxylic Acid Homodimers: Hydrogen Bonds and Atmospheric Implications. Journal of Physical Chemistry A, 2016, 120, 2342-2349.	2.5	14
35	Noniterative corrections to equationâ€ofâ€motion coupledâ€cluster excited state energies based on the reduced method of moments of coupled cluster equations. International Journal of Quantum Chemistry, 2008, 108, 2178-2190.	2.0	13
36	Interactions of Cl^{â^'} and OH Radical in Aqueous Solution. Journal of Physical Chemistry A, 2009, 113, 8823-8825.	2.5	13

#	Article	IF	Citations
37	CH₂Cl₂ + OH^{â˙™} Reaction in Aqueous Solution: A Combined Quantum Mechanical and Molecular Mechanics Study. Journal of Physical Chemistry A, 2011, 115, 1380-1384.	2.5	13
38	Decomposition of amino diazeniumdiolates (NONOates): Molecular mechanisms. Journal of Inorganic Biochemistry, 2014, 141, 28-35.	3.5	12
39	Site density models of inhomogeneous classical molecular liquids. Journal of Statistical Mechanics: Theory and Experiment, 2018, 2018, 093201.	2.3	12
40	Calculations of Molecular Properties in Hybrid Coupled-Cluster and Molecular Mechanics Approach. Journal of Physical Chemistry A, 2007, 111, 5492-5498.	2.5	10
41	Negative ion photoelectron spectra of ISO3â€“, IS2O3â€“, and IS2O4â€“ intermediates formed in interfacial reactions of ozone and iodide/sulfite aqueous microdroplets. Journal of Chemical Physics, 2016, 145, 214310.	3.0	10
42	Photoelectron spectroscopy of solvated dicarboxylate and alkali metal ion clusters, M+[O2C(CH2)2CO2]2â˙™ [H2O]n (M = Na, K; n = 1â€“6). Physical Chemistry Chemical Physics, 2018, 20, 29051-29060.	2.8	10
43	Chemical bond effects in classical site density functional theory of inhomogeneous molecular liquids. Journal of Chemical Physics, 2020, 152, 041101.	3.0	10
44	FIRST PRINCIPLES MOLECULAR DYNAMICS SIMULATIONS USING DENSITY-FUNCTIONAL THEORY. , 2002, , 1684-1734.		9
45	Structural and Mechanistic Analysis through Electronic Spectra: Aqueous Hyponitrite Radical (N₂O₂^{â€“}) and Nitrosyl Hyponitrite Anion (N₃O₃^{â€“}). Journal of Physical Chemistry A, 2011, 115, 12004-12010.	2.5	9
46	Advances in Scalable Computational Chemistry. Annual Reports in Computational Chemistry, 2011, 7, 151-177.	1.7	8
47	Sulfuric acid and aromatic carboxylate clusters H2SO4Â·ArCOOâ˙™: Structures, properties, and their relevance to the initial aerosol nucleation. International Journal of Mass Spectrometry, 2019, 439, 27-33.	1.5	8
48	Renormalized site density functional theory. Journal of Statistical Mechanics: Theory and Experiment, 2021, 2021, 033205.	2.3	7
49	Renormalized site density functional theory for models of ion hydration. Journal of Chemical Physics, 2021, 155, 064501.	3.0	6
50	CDFTPY: A python package for performing classical density functional theory calculations for molecular liquids. Computer Physics Communications, 2022, 276, 108338.	7.5	6
51	Water assisted reaction mechanism of OHâ˙™ with CCl4 in aqueous solution â€“ Hybrid quantum mechanical and molecular mechanics investigation. Chemical Physics Letters, 2013, 559, 30-34.	2.6	5
52	Examining the Amine Functionalization in Dicarboxylates: Photoelectron Spectroscopy and Theoretical Studies of Aspartate and Glutamate. Journal of Physical Chemistry A, 2014, 118, 5256-5262.	2.5	5
53	Distonic radical anion species in cysteine oxidation processes. Physical Chemistry Chemical Physics, 2020, 22, 17554-17558.	2.8	5
54	Site Density Functional Theory and Structural Bioinformatics Analysis of the SARS-CoV Spike Protein and hACE2 Complex. Molecules, 2022, 27, 799.	3.8	5

#	Article	IF	Citations
55	Structure of Low-Lying Excited States of Guanine in DNA and Solution: Combined Molecular Mechanics and High-Level Coupled Cluster Studies. Research Letters in Physical Chemistry, 2007, 2007, 1-5.	0.3	4
56	Combined quantumâ€mechanical molecular mechanics calculations with NWChem and AMBER: Excited state properties of green fluorescent protein chromophore analogue in aqueous solution. Journal of Computational Chemistry, 2017, 38, 1631-1639.	3.3	3
57	Photoelectron Spectroscopy and Theoretical Study on Monosolvated Cyanate Analogue Clusters ECX^{â€“}Â·Sol (ECX^{â€“} = NCSe^{â€“}, AsCSe^{â€“}, and) Tj ETQq1 1 0.784314 rgBT /Ov 125, 3928-3935.	2.5	3