# Marat Valiev

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Site Density Functional Theory and Structural Bioinformatics Analysis of the SARS-CoV Spike Protein and hACE2 Complex. Molecules, 2022, 27, 799. | 3.8 | 5 |
| 2 | CDFTPY: A python package for performing classical density functional theory calculations for molecular liquids. Computer Physics Communications, 2022, 276, 108338. | 7.5 | 6 |
| 3 | Renormalized site density functional theory. Journal of Statistical Mechanics: Theory and Experiment, 2021, 2021, 033205. | 2.3 | 7 |
| 4 | From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998. | 47.7 | 39 |
| 5 | Photoelectron Spectroscopy and Theoretical Study on Monosolvated Cyanate Analogue Clusters ECX<sup>â€“</sup>·Sol (ECX<sup>â€“</sup> = NCSe<sup>â€“</sup>, AsCSe<sup>â€“</sup>, and) Tj ETQq1 1 0.784314 rgBT /Over 125, 3928-3935. | 2.5 | 3 |
| 6 | Renormalized site density functional theory for models of ion hydration. Journal of Chemical Physics, 2021, 155, 064501. | 3.0 | 6 |
| 7 | Distonic radical anion species in cysteine oxidation processes. Physical Chemistry Chemical Physics, 2020, 22, 17554-17558. | 2.8 | 5 |
| 8 | NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102. | 3.0 | 425 |
| 9 | 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 |
| 10 | Chemical bond effects in classical site density functional theory of inhomogeneous molecular liquids. Journal of Chemical Physics, 2020, 152, 041101. | 3.0 | 10 |
| 11 | 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 |
| 12 | 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 |
| 13 | Site density models of inhomogeneous classical molecular liquids. Journal of Statistical Mechanics: Theory and Experiment, 2018, 2018, 093201. | 2.3 | 12 |
| 14 | 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 |
| 15 | 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 |
| 16 | Formation of (HCOO<sup>â€“</sup>)(H<sub>2</sub>SO<sub>4</sub>) Anion Clusters: Violation of Gas-Phase Acidity Predictions. Journal of the American Chemical Society, 2017, 139, 11321-11324. | 13.7 | 22 |
| 17 | Deprotonated Dicarboxylic Acid Homodimers: Hydrogen Bonds and Atmospheric Implications. Journal of Physical Chemistry A, 2016, 120, 2342-2349. | 2.5 | 14 |
| 18 | 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 |

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|---|---|---|---|
| 19 | How Anion Chaotrope Changes the Local Structure of Water: Insights from Photoelectron Spectroscopy and Theoretical Modeling of SCN<sup>â€“</sup> Water Clusters. Journal of Physical Chemistry B, 2016, 120, 1518-1525. | 2.6 | 20 |
| 20 | 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 |
| 21 | 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 |
| 22 | Decomposition of amino diazeniumdiolates (NONOates): Molecular mechanisms. Journal of Inorganic Biochemistry, 2014, 141, 28-35. | 3.5 | 12 |
| 23 | 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 |
| 24 | Simulating Ru L<sub>3</sub>-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 |
| 25 | Communication: Solute anisotropy effects in hydrated anion and neutral clusters. Journal of Chemical Physics, 2013, 138, 031101. | 3.0 | 22 |
| 26 | 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 |
| 27 | Study of Ion Specific Interactions of Alkali Cations with Dicarboxylate Dianions. Journal of Physical Chemistry A, 2012, 116, 2055-2061. | 2.5 | 24 |
| 28 | Hybrid Quantum Mechanical and Molecular Mechanics Study of the S<sub>N</sub>2 Reaction of CCl<sub>4</sub> + OH<sup>â€“</sup> 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 |
| 29 | CH<sub>2</sub>Cl<sub>2</sub> + OH<sup>â^'</sup> Reaction in Aqueous Solution: A Combined Quantum Mechanical and Molecular Mechanics Study. Journal of Physical Chemistry A, 2011, 115, 1380-1384. | 2.5 | 13 |
| 30 | Hybrid Quantum Mechanical/Molecular Mechanics Study of the S<sub>N</sub>2 Reaction of CH<sub>3</sub>Cl+OH<sup>â€“</sup> in Water. Journal of Physical Chemistry A, 2011, 115, 12047-12052. | 2.5 | 41 |
| 31 | Structural and Mechanistic Analysis through Electronic Spectra: Aqueous Hyponitrite Radical ($N_2O_2^{-}$) and Nitrosyl Hyponitrite Anion ($N_3O_3^{-}$). Journal of Physical Chemistry A, 2011, 115, 12004-12010. | 2.5 | 9 |
| 32 | NWChem: scalable parallel computational chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 888-894. | 14.6 | 27 |
| 33 | Advances in Scalable Computational Chemistry. Annual Reports in Computational Chemistry, 2011, 7, 151-177. | 1.7 | 8 |
| 34 | NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489. | 7.5 | 4,740 |
| 35 | Vertical Ionization Potentials of Nucleobases in a Fully Solvated DNA Environment. Journal of Physical Chemistry B, 2010, 114, 5886-5894. | 2.6 | 69 |
| 36 | Interactions of Cl<sup>â^'</sup> and OH Radical in Aqueous Solution. Journal of Physical Chemistry A, 2009, 113, 8823-8825. | 2.5 | 13 |

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|---|---|---|---|
| 37 | A Dianionic Phosphorane Intermediate and Transition States in an Associative A<sub>N</sub>+D<sub>N</sub> Mechanism for the RibonucleaseA Hydrolysis Reaction. Journal of the American Chemical Society, 2009, 131, 3869-3871. | 13.7 | 32 |
| 38 | 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 |
| 39 | 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 |
| 40 | 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 |
| 41 | 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 |
| 42 | On the Electronically Excited States of Uracil. Journal of Physical Chemistry A, 2008, 112, 9983-9992. | 2.5 | 115 |
| 43 | 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 |
| 44 | Application of High-Level Iterative Coupled-Cluster Methods to the Cytosine Molecule. Journal of Physical Chemistry A, 2008, 112, 5538-5541. | 2.5 | 14 |
| 45 | 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 |
| 46 | Calculations of Molecular Properties in Hybrid Coupled-Cluster and Molecular Mechanics Approach. Journal of Physical Chemistry A, 2007, 111, 5492-5498. | 2.5 | 10 |
| 47 | 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 |
| 48 | 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 |
| 49 | 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 |
| 50 | 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 |
| 51 | Fast electron correlation methods for molecular clusters in the ground and excited states. Molecular Physics, 2005, 103, 2255-2265. | 1.7 | 137 |
| 52 | 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 |
| 53 | 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 |
| 54 | FIRST PRINCIPLES MOLECULAR DYNAMICS SIMULATIONS USING DENSITY-FUNCTIONAL THEORY. , 2002, , 1684-1734. | | 9 |

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|---|---|---|---|
| 55 | Parallel implementation of the projector augmented plane wave method for charged systems. Computer Physics Communications, 2002, 143, 11-28. | 7.5 | 35 |
| 56 | The Projector-Augmented Plane Wave Method Applied to Molecular Bonding. Journal of Physical Chemistry A, 1999, 103, 10588-10601. | 2.5 | 27 |
| 57 | Density-functional theory of one-electron propagators. Physics Letters, Section A: General, Atomic and Solid State Physics, 1997, 227, 265-270. | 2.1 | 23 |