Ruslan Kevorkyants

List of Publications by Year
in descending order

37 papers	692 citations	759233 12 h-index	552781 26 g-index
37 all docs	37 docs citations	37 times ranked	1132 citing authors

#	Article	IF	Citations
1	Self-Assembled Organic Nanowires for High Power Density Lithium Ion Batteries. Nano Letters, 2014, 14, 1596-1602.	9.1	187
2	Interaction between n-Alkane Chains:â€‰ Applicability of the Empirically Corrected Density Functional Theory for Van der Waals Complexes. Journal of Chemical Theory and Computation, 2007, 3, 755-763.	5.3	94
3	Porphyrin Traps Its Terminator! Concerted and Stepwise Porphyrin Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450. Angewandte Chemie - International Edition, 2004, 43, 1129-1132.	13.8	60
4	Interaction energies in hydrogen-bonded systems: A testing ground for subsystem formulation of density-functional theory. Journal of Chemical Physics, 2006, 124, 024104.	3.0	48
5	Microstructural analysis and optical properties of the halide double perovskite Cs2BiAgBr6 single crystals. Chemical Physics Letters, 2018, 694, 18-22.	2.6	42
6	Low Inhomogeneous Broadening of Excitonic Resonance in MAPbBr₃ Single Crystals. Journal of Physical Chemistry Letters, 2018, 9, 302-305.	4.6	27
7	FDE-vdW: A van der Waals inclusive subsystem density-functional theory. Journal of Chemical Physics, 2014, 141, 044127.	3.0	24
8	Pyridinium lead tribromide and pyridinium lead triiodide: quasi-one-dimensional perovskites with an optically active aromatic Ï€-system. Dalton Transactions, 2018, 47, 16313-16319.	3.3	24
9	Hybrid Organicâ€“Inorganic Halide Postâ€Perovskite 3â€Cyanopyridinium Lead Tribromide for Optoelectronic Applications. Advanced Functional Materials, 2021, 31, 2102338.	14.9	18
10	The effect of organic cations on the electronic, optical and luminescence properties of 1D piperidinium, pyridinium, and 3-hydroxypyridinium lead trihalides. Dalton Transactions, 2020, 49, 4390-4403.	3.3	16
11	Calculating Hyperfine Couplings in Large Ionic Crystals Containing Hundreds of QM Atoms: Subsystem DFT Is the Key. Journal of Physical Chemistry B, 2013, 117, 13967-13974.	2.6	15
12	Revisiting the BaBiO3 semiconductor photocatalyst: synthesis, characterization, electronic structure, and photocatalytic activity. Photochemical and Photobiological Sciences, 2021, 20, 1147-1160.	2.9	13
13	The origin of 1560 cmâ^'1 band in experimental IR spectra of water adsorbed on TiO2 surface: Ab initio assessment. Chemical Physics Letters, 2016, 662, 97-101.	2.6	12
14	Materials synthesis, characterization and DFT calculations of the visible-light-active perovskite-like barium bismuthate Ba_{1.264(4)}Bi_{1.971(4)}O₄ photocatalyst. Journal of Materials Chemistry C, 2020, 8, 3509-3519.	5.5	12
15	The performance of the semi-empirical AM1 method on small and nanometre-sized N2O clusters. Physical Chemistry Chemical Physics, 2004, 6, 4939-4949.	2.8	11
16	The T-shaped KrI2(ion-pair states) van der Waals complexes. Chemical Physics Letters, 2017, 684, 357-362.	2.6	11
17	¹³C NMR chemical shift calculations of charged surfactants in water â€" A combined density functional theory (DFT) and molecular dynamics (MD) methodological study. Canadian Journal of Chemistry, 2013, 91, 529-537.	1.1	9
18	Effect of Composition on the Optical and Photocatalytic Properties of Visible Light Responsive Materials Bi_{26â€“x}Mg_xO₄₀. Inorganic Chemistry, 2020, 59, 8173-8183.	4.0	9

#	Article	IF	Citations
19	Synthesis, characterization, optoelectronic and photocatalytic properties of Sr2Bi2O5/SrCO3 and Sr3Bi2O6/SrCO3 heterostructures with varying SrCO3 content. Chemosphere, 2021, 267, 129229.	8.2	9
20	DFT study of molecular hydrogen interaction with photoexcited TiO2 surface: Nanocluster model. Chemical Physics Letters, 2015, 639, 225-229.	2.6	6
21	Ab Initio Insight into Mechanisms of Ozone Interaction with a Surface of Dehydrated Nanocrystalline TiO₂. Langmuir, 2020, 36, 1930-1936.	3.5	6
22	Ab initio R1 mechanism of photostimulated oxygen isotope exchange reaction on a defect TiO2 surface: The case of terminal oxygen atom exchange. Applied Surface Science, 2017, 403, 342-346.	6.1	5
23	Hybrid organic-inorganic lead and tin halide perovskites with saturated heterocyclic cations (CH2)nNH2+ and (CH2)nOH+, (n = 2â€“6): Ab initio study. Computational Materials Science, 2017, 138, 99-104.	3.0	5
24	Modulating electronic properties of pyridinium lead halide perovskites via fluorinated methyl substituents. Materials Chemistry and Physics, 2021, 273, 125139.	4.0	5
25	The valence and ion-pair states of the N2I2 van der Waals complex. Chemical Physics Letters, 2019, 714, 213-218.	2.6	4
26	Hybrid lead triiodide perovskites with unsaturated heterocyclic cations containing N, O, and S atoms: Ab initio study. Journal of Solid State Chemistry, 2020, 282, 121082.	2.9	4
27	Poly â€“NÂ=ÂNâ€“ linked 1,5-dihydro-1,5-diazocine, the two-dimensional polymer withDirac insulatorproperties:ab initiostudy. Molecular Simulation, 2012, 38, 886-891.	2.0	3
28	Modulating optoelectronic properties of organo-metal halide perovskites with unsaturated heterocyclic cations via ring substitution. Journal of Physics and Chemistry of Solids, 2019, 135, 109078.	4.0	3
29	The structure and aromaticity of 1,4 and 1,5 dihydro diazocine, dioxocine, hydro oxazocine: ab initio CCSD(T) singlet potential energy surface study. Tetrahedron Letters, 2016, 57, 340-344.	1.4	2
30	Novel hybrid semiconducting lead and tin halide perovskites with saturated heterocyclic cations (CH2)nPH2+ and (CH2)nSH+, (n=2â€“6): Ab initio study. Materials Chemistry and Physics, 2019, 229, 387-391.	4.0	2
31	One-Electron Equations for Embedded Electron Density and Their Applications to Study Electronic Structure of Atoms and Molecules in Condensed Phase. Chimia, 2005, 59, 488-492.	0.6	2
32	Photoionisation study of Xe.CF4 and Kr.CF4 van-der-Waals molecules. Journal of Chemical Physics, 2016, 144, 184305.	3.0	1
33	Novel 3D photoactive direct bandgap perovskites CsBiPbX6: Ab initio structure and electronic properties. Computational Materials Science, 2020, 183, 109819.	3.0	1
34	The Study of Photoactive Materials. Reviews and Advances in Chemistry, 2020, 10, 73-111.	0.5	1
35	Crystal and electronic structure of the sub-stoichiometric photocatalyst Cu4Se6: DFT study. Journal of Physics and Chemistry of Solids, 2022, 162, 110529.	4.0	1
36	Ionization of Kr.CF₄ and Xe.CF₄ van der Waals clusters: from face to vertex geometry. Journal of Physics: Conference Series, 2015, 635, 112056.	0.4	0

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37	Electronic-state-driven adsorption of O2 on a nanocrystalline TiO2 under â€˜darkâ€™ and UV-irradiation conditions: Ab initio study. Chemical Physics Letters, 2018, 698, 97-101.	2.6	0