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	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
2	Synthesis, characterization, optoelectronic and photocatalytic properties of Sr2Bi2O5/SrCO3 and Sr3Bi2O6/SrCO3 heterostructures with varying SrCO3 content. Chemosphere, 2021, 267, 129229.	8.2	9
3	Hybrid Organicâ€“Inorganic Halide Postâ€Perovskite 3â€Cyanopyridinium Lead Tribromide for Optoelectronic Applications. Advanced Functional Materials, 2021, 31, 2102338.	14.9	18
4	Revisiting the BaBiO3 semiconductor photocatalyst: synthesis, characterization, electronic structure, and photocatalytic activity. Photochemical and Photobiological Sciences, 2021, 20, 1147-1160.	2.9	13
5	Modulating electronic properties of pyridinium lead halide perovskites via fluorinated methyl substituents. Materials Chemistry and Physics, 2021, 273, 125139.	4.0	5
6	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
7	Novel 3D photoactive direct bandgap perovskites CsBiPbX6: Ab initio structure and electronic properties. Computational Materials Science, 2020, 183, 109819.	3.0	1
8	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
9	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
10	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
11	Ab Initio Insight into Mechanisms of Ozone Interaction with a Surface of Dehydrated Nanocrystalline TiO₂. Langmuir, 2020, 36, 1930-1936.	3.5	6
12	The Study of Photoactive Materials. Reviews and Advances in Chemistry, 2020, 10, 73-111.	0.5	1
13	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
14	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
15	The valence and ion-pair states of the N2I2 van der Waals complex. Chemical Physics Letters, 2019, 714, 213-218.	2.6	4
16	Microstructural analysis and optical properties of the halide double perovskite Cs2BiAgBr6 single crystals. Chemical Physics Letters, 2018, 694, 18-22.	2.6	42
17	Low Inhomogeneous Broadening of Excitonic Resonance in MAPbBr₃ Single Crystals. Journal of Physical Chemistry Letters, 2018, 9, 302-305.	4.6	27
18	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

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19	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
20	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
21	The T-shaped KrI2(ion-pair states) van der Waals complexes. Chemical Physics Letters, 2017, 684, 357-362.	2.6	11
22	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
23	Photoionisation study of Xe.CF4 and Kr.CF4 van-der-Waals molecules. Journal of Chemical Physics, 2016, 144, 184305.	3.0	1
24	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
25	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
26	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
27	DFT study of molecular hydrogen interaction with photoexcited TiO2 surface: Nanocluster model. Chemical Physics Letters, 2015, 639, 225-229.	2.6	6
28	FDE-vdW: A van der Waals inclusive subsystem density-functional theory. Journal of Chemical Physics, 2014, 141, 044127.	3.0	24
29	Self-Assembled Organic Nanowires for High Power Density Lithium Ion Batteries. Nano Letters, 2014, 14, 1596-1602.	9.1	187
30	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
31	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
32	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
33	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
34	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
35	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
36	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

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37	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