Dmitry Bocharov

List of Publications by Year
in descending order

42	541	623734 14	677142 22
papers	citations	h-index	g-index

43	43	43	572
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A comprehensive study of structure and properties of nanocrystalline zinc peroxide. Journal of Physics and Chemistry of Solids, 2022, 160, 110318.	4.0	6
2	Validation of moment tensor potentials for fcc and bcc metals using EXAFS spectra. Computational Materials Science, 2022, 210, 111028.	3.0	5
3	CO2 and CH2 Adsorption on Copper-Decorated Graphene: Predictions from First Principle Calculations. Crystals, 2022, 12, 194.	2.2	9
4	Influence of Au, Ag, and Cu Adatoms on Optical Properties of TiO2 (110) Surface: Predictions from RT-TDDFT Calculations. Crystals, 2022, 12, 452.	2.2	4
5	Excited States Calculations of MoS2@ZnO and WS2@ZnO Two-Dimensional Nanocomposites for Water-Splitting Applications. Energies, 2022, 15, 150.	3.1	14
6	Ab Initio Computations of O and AO as well as ReO2, WO2 and BO2-Terminated ReO3, WO3, BaTiO3, SrTiO3 and BaZrO3 (001) Surfaces. Symmetry, 2022, 14, 1050.	2.2	23
7	2D Slab Models of Nanotubes Based on Tetragonal TiO2 Structures: Validation over a Diameter Range. Nanomaterials, 2021, 11, 1925.	4.1	4
8	Study of High-Temperature Behaviour of ZnO by Ab Initio Molecular Dynamics Simulations and X-ray Absorption Spectroscopy. Materials, 2021, 14, 5206.	2.9	3
9	Water Splitting on Multifaceted SrTiO3 Nanocrystals: Computational Study. Catalysts, 2021, 11, 1326.	3.5	7
10	Interpretation of the Cu K-edge EXAFS spectra of Cu3N using ab initio molecular dynamics. Radiation Physics and Chemistry, 2020, 175, 108100.	2.8	5
11	Ab initio molecular dynamics simulations of negative thermal expansion in ScF3: The effect of the supercell size. Computational Materials Science, 2020, 171, 109198.	3.0	15
12	2D slab models of TiO2 nanotubes for simulation of water adsorption: Validation over a diameter range. Results in Physics, 2020, 19, 103527.	4.1	4
13	Ab Initio Calculations on the Electronic Structure and Photocatalytic Properties of Twoâ€Dimensional WS₂ (0001) Nanolayers of Varying Thickness. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800253.	2.4	16
14	Water Adsorption on Clean and Defective Anatase TiO2 (001) Nanotube Surfaces: A Surface Science Approach. Journal of Physical Chemistry B, 2018, 122, 5432-5440.	2.6	20
15	Validation of a constrained 2D slab model for water adsorption simulation on 1D periodic TiO2 nanotubes. Computational Condensed Matter, 2018, 15, 69-78.	2.1	7
16	Quantum chemical simulations of titanium dioxide nanotubes used for photocatalytic water splitting. Journal of Surface Investigation, 2017, 11, 78-86.	0.5	3
17	First principles modeling of 3d-metal doped three-layer fluorite-structured TiO2 (4,4) nanotube to be used for photocatalytic hydrogen production. Vacuum, 2017, 146, 562-569.	3.5	13
18	Doped 1D Nanostructures of Transitionâ€metal Oxides: Firstâ€principles Evaluation of Photocatalytic Suitability. Israel Journal of Chemistry, 2017, 57, 461-476.	2.3	15

#	Article	IF	Citations
19	First-principles calculations on Fe-Pt nanoclusters of various morphologies. Scientific Reports, 2017, 7, 10579.	3.3	2
20	Analysis of the U L 3 -edge X-ray absorption spectra in UO 2 using molecular dynamics simulations. Progress in Nuclear Energy, 2017, 94, 187-193.	2.9	8
21	First Principle Evaluation of Photocatalytic Suitability for TiO2-Based Nanotubes. , 2016, , .		1
22	Interpretation of the U L₃-edge EXAFS in uranium dioxide using molecular dynamics and density functional theory simulations. Journal of Physics: Conference Series, 2016, 712, 012091.	0.4	1
23	Electronic structure of cubic ScF3 from first-principles calculations. Low Temperature Physics, 2016, 42, 556-560.	0.6	9
24	Interpretation of unexpected behavior of infrared absorption spectra of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ScF</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> in the quasiharmonic approximation. Physical Review B, 2016, 93, .	3.2	17
25	Local structure of perovskites ReO₃and ScF₃with negative thermal expansion: interpretation beyond the quasiharmonic approximation. Journal of Physics: Conference Series, 2016, 712, 012013.	0.4	3
26	Ab initio molecular dynamics simulations of the Sc K-edge EXAFS of scandium trifluoride. Journal of Physics: Conference Series, 2016, 712, 012009.	0.4	4
27	Ab initio calculations of doped TiO2 anatase (101) nanotubes for photocatalytical water splitting applications. Materials Science in Semiconductor Processing, 2016, 42, 138-141.	4.0	13
28	Ab initiosimulations on N and S co-doped titania nanotubes for photocatalytic applications. Physica Scripta, 2015, 90, 094013.	2.5	10
29	C-, N-, S-, and Fe-Doped TiO₂ and SrTiO₃ Nanotubes for Visible-Light-Driven Photocatalytic Water Splitting: Prediction from First Principles. Journal of Physical Chemistry C, 2015, 119, 18686-18696.	3.1	104
30	Local Structure Studies of Ti for SrTi¹⁶O₃and SrTi¹⁸O₃by Advanced X-ray Absorption Spectroscopy Data Analysis. Ferroelectrics, 2015, 485, 42-52.	0.6	3
31	Local structure studies of SrTi¹⁶O₃and SrTi¹⁸O₃. Physica Scripta, 2014, 89, 044002.	2.5	4
32	Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride. Journal of Nuclear Materials, 2013, 435, 102-106.	2.7	18
33	Electronic charge redistribution in LaAlO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>(001) thin films deposited at SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>(001) substrate: First-principles analysis and the role of stoichiometry. Physical Review B, 2012, 86, .	3.2	18
34	Ab initiomodelling of UN grain boundary interfaces. IOP Conference Series: Materials Science and Engineering, 2012, 38, 012058.	0.6	0
35	Ab initio modeling of oxygen impurity atom incorporation into uranium mononitride surface and sub-surface vacancies. Journal of Nuclear Materials, 2011, 416, 200-204.	2.7	33
36	DFT calculations of point defects on UN(001) surface. Surface Science, 2011, 605, 396-400.	1.9	26

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37	First principles calculations of oxygen adsorption on the UN(001) surface. Surface Science, 2009, 603, 50-53.	1.9	22
38	Chemisorption of a molecular oxygen on the UN(001) surface: Ab initio calculations. Journal of Nuclear Materials, 2009, 393, 504-507.	2.7	25
39	Methods of electron microdiffraction and X-ray analysis in structure study of nanodisperse partially stabilized ZrO2 powders. Journal of Surface Investigation, 2009, 3, 464-467.	0.5	2
40	A firstâ€principles DFT study of UN bulk and (001) surface: Comparative LCAO and PW calculations. Journal of Computational Chemistry, 2008, 29, 2079-2087.	3.3	40
41	<title>Quantum chemistry studies of the O K-edge x-ray absorption in WO<formula><inf><roman>3</roman></inf></formula> and AWO<formula><inf><roman>3</roman></inf></formula></title>. Proceedings of SPIE, 2008, . .	0.8	1
42	Negative thermal expansion of ScF₃: first principles vs empirical molecular dynamics. IOP Conference Series: Materials Science and Engineering, 0, 503, 012001.	0.6	4