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	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
2	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
3	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
4	DFT calculations of point defects on UN(001) surface. Surface Science, 2011, 605, 396-400.	1.9	26
5	Chemisorption of a molecular oxygen on the UN(001) surface: Ab initio calculations. Journal of Nuclear Materials, 2009, 393, 504-507.	2.7	25
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	First principles calculations of oxygen adsorption on the UN(001) surface. Surface Science, 2009, 603, 50-53.	1.9	22
8	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
9	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
10	Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride. Journal of Nuclear Materials, 2013, 435, 102-106.	2.7	18
11	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
12	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
13	Doped 1D Nanostructures of Transitionâ€metal Oxides: Firstâ€principles Evaluation of Photocatalytic Suitability. Israel Journal of Chemistry, 2017, 57, 461-476.	2.3	15
14	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
15	Excited States Calculations of MoS2@ZnO and WS2@ZnO Two-Dimensional Nanocomposites for Water-Splitting Applications. Energies, 2022, 15, 150.	3.1	14
16	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
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	Ab initiosimulations on N and S co-doped titania nanotubes for photocatalytic applications. Physica Scripta, 2015, 90, 094013.	2.5	10

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19	Electronic structure of cubic ScF3 from first-principles calculations. Low Temperature Physics, 2016, 42, 556-560.	0.6	9
20	CO2 and CH2 Adsorption on Copper-Decorated Graphene: Predictions from First Principle Calculations. Crystals, 2022, 12, 194.	2.2	9
21	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
22	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
23	Water Splitting on Multifaceted SrTiO3 Nanocrystals: Computational Study. Catalysts, 2021, 11, 1326.	3.5	7
24	A comprehensive study of structure and properties of nanocrystalline zinc peroxide. Journal of Physics and Chemistry of Solids, 2022, 160, 110318.	4.0	6
25	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
26	Validation of moment tensor potentials for fcc and bcc metals using EXAFS spectra. Computational Materials Science, 2022, 210, 111028.	3.0	5
27	Local structure studies of SrTi¹⁶O₃and SrTi¹⁸O₃. Physica Scripta, 2014, 89, 044002.	2.5	4
28	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
29	Negative thermal expansion of ScF₃: first principles vs empirical molecular dynamics. IOP Conference Series: Materials Science and Engineering, 0, 503, 012001.	0.6	4
30	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
31	2D Slab Models of Nanotubes Based on Tetragonal TiO2 Structures: Validation over a Diameter Range. Nanomaterials, 2021, 11, 1925.	4.1	4
32	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
33	Local Structure Studies of Ti for SrTi¹⁶O₃and SrTi¹⁸O₃by Advanced X-ray Absorption Spectroscopy Data Analysis. Ferroelectrics, 2015, 485, 42-52.	0.6	3
34	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
35	Quantum chemical simulations of titanium dioxide nanotubes used for photocatalytic water splitting. Journal of Surface Investigation, 2017, 11, 78-86.	0.5	3
36	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

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37	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
38	First-principles calculations on Fe-Pt nanoclusters of various morphologies. Scientific Reports, 2017, 7, 10579.	3.3	2
39	<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
40	First Principle Evaluation of Photocatalytic Suitability for TiO2-Based Nanotubes. , 2016, , .		1
41	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
42	Ab initiomodelling of UN grain boundary interfaces. IOP Conference Series: Materials Science and Engineering, 2012, 38, 012058.	0.6	0