D V Gryaznov

List of Publications by Year
in descending order

58	1,179	394421	395702
papers	citations	19 h-index	33 g-index

58	58	58	1235
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Single oxygen vacancy in BaCoO3: Hybrid DFT calculations and local site symmetry approach. Solid State Ionics, 2022, 375, 115835.	2.7	0
2	Oxygen Vacancy Formation and Migration within the Antiphase Boundaries in Lanthanum Scandate-Based Oxides: Computational Study. Materials, 2022, 15, 2695.	2.9	0
3	Electrochemical Performance of NASICON-structured Na3-x V2-xTix(PO4)3 (0.0 < x < 1.0) as aqueous Na-ion battery positive electrodes. Electrochimica Acta, 2022, 424, 140580.	5.2	6
4	The local atomic structure and thermoelectric properties of Ir-doped ZnO: hybrid DFT calculations and XAS experiments. Journal of Materials Chemistry C, 2021, 9, 4948-4960.	5.5	7
5	BaCoO3 monoclinic structure and chemical bonding analysis: hybrid DFT calculations. Physical Chemistry Chemical Physics, 2021, 23, 17493-17501.	2.8	4
6	Small radius electron and hole polarons in PbX₂ (X = F, Cl, Br) crystals: a computational study. Journal of Materials Chemistry C, 2021, 9, 16536-16544.	5.5	8
7	Peculiarities of Phase Formation in Mn-Based Na Superlonic Conductor (NaSICon) Systems: The Case of Na_{1+2x}Mn_xTi_{2â€“x}(PO₄)₃ (0.0 â‰¤ x â‰¤ 1.5). Chemistry of Materials, 2021, 33, 8394-8403.	6.7	9
8	Hybrid density functional calculations of hyperfine coupling tensor for hole-type defects in MgAl2O4. Nuclear Instruments & Methods in Physics Research B, 2020, 464, 60-64.	1.4	15
9	Atomic, electronic and magnetic structure of an oxygen interstitial in neutron-irradiated Al2O3 single crystals. Scientific Reports, 2020, 10, 15852.	3.3	18
10	First principles calculations of the vibrational properties of single and dimer F-type centers in corundum crystals. Journal of Chemical Physics, 2020, 153, 134107.	3.0	5
11	Hybrid density functional theoretical study of NASICON-type Na_xTi₂(PO₄)₃ (x = 1â€“4). Physical Chemistry Chemical Physics, 2020, 22, 11861-11870.	2.8	6
12	Interdependence of Oxygenation and Hydration in Mixed-Conducting (Ba,Sr)FeO_{3â^’Î´} Perovskites Studied by Density Functional Theory. Journal of Physical Chemistry C, 2020, 124, 11780-11789.	3.1	24
13	Ab initio calculations of pure and Co+2-doped MgF2 crystals. Nuclear Instruments & Methods in Physics Research B, 2020, 470, 10-14.	1.4	5
14	First principles calculations on CeO2 doped with Tb3+ ions. Optical Materials, 2019, 90, 76-83.	3.6	3
15	Interface-induced enhancement of piezoelectricity in the (SrTiO₃)_m/(BaTiO₃)_{Mâ’m} superlattice for energy harvesting applications. Physical Chemistry Chemical Physics, 2019, 21, 23541-23551.	2.8	9
16	First Principles Simulations on Migration Paths of Oxygen Interstitials in MgAl₂O₄. Physica Status Solidi (B): Basic Research, 2019, 256, 1800282.	1.5	7
17	Ab initio simulations on charged interstitial oxygen migration in corundum. Nuclear Instruments & Methods in Physics Research B, 2018, 435, 74-78.	1.4	14
18	Dopant solubility in ceria: alloy thermodynamics combined with the DFT+U calculations. Solid State Ionics, 2018, 325, 258-264.	2.7	1

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19	Use of site symmetry in supercell models of defective crystals: polarons in CeO₂. Physical Chemistry Chemical Physics, 2017, 19, 8340-8348.	2.8	20
20	First-principles calculations of oxygen interstitials in corundum: a site symmetry approach. Physical Chemistry Chemical Physics, 2017, 19, 25245-25251.	2.8	19
21	Ab initio modelling of oxygen vacancies and protonic defects in La_{1â^'x}Sr_xFeO_{3â^'Î´} perovskite solid solutions. Journal of Materials Chemistry A, 2016, 4, 13093-13104.	10.3	33
22	Charged oxygen interstitials in corundum: first principles simulations. Physica Status Solidi C: Current Topics in Solid State Physics, 2016, 13, 932-936.	0.8	5
23	Confinement effects for the F center in non-stoichiometric BaZrO₃ ultrathin films. Physica Status Solidi (B): Basic Research, 2015, 252, 139-143.	1.5	6
24	Thermodynamic properties of neutral and charged oxygen vacancies in BaZrO₃ based on first principles phonon calculations. Physical Chemistry Chemical Physics, 2015, 17, 20765-20774.	2.8	47
25	Comparison of Permeation Measurements and Hybrid Density-Functional Calculations on Oxygen Vacancy Transport in Complex Perovskite Oxides. Journal of Physical Chemistry C, 2014, 118, 29542-29553.	3.1	25
26	Oxygen vacancy formation energies in Sr-doped complex perovskites: ab initio thermodynamic study. Solid State Ionics, 2014, 254, 11-16.	2.7	26
27	Theoretical modeling of antiferrodistortive phase transition for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>SrTi</mml:mtext><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>ultrathin films. Physical Review B, 2013, 88, .	3.2	13
28	Ab initio study of phase competition in (La1â^'c,Src)CoO3 solid solutions. Solid State Ionics, 2013, 230, 32-36.	2.7	15
29	Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride. Journal of Nuclear Materials, 2013, 435, 102-106.	2.7	18
30	A Comparative Ab Initio Thermodynamic Study of Oxygen Vacancies in ZnO and SrTiO₃: Emphasis on Phonon Contribution. Journal of Physical Chemistry C, 2013, 117, 13776-13784.	3.1	72
31	The first-principles treatment of the electron-correlation and spinâ€“orbital effects in uranium mononitride nuclear fuels. Physical Chemistry Chemical Physics, 2012, 14, 4482.	2.8	70
32	Jahn-Teller effect in the phonon properties of defective 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>from first principles. Physical Review B, 2012, 85, .	3.2	51
33	Ab initiomodelling of UN grain boundary interfaces. IOP Conference Series: Materials Science and Engineering, 2012, 38, 012058.	0.6	0
34	Confinement effects for ionic carriers in SrTiO₃ultrathin films: first-principles calculations of oxygen vacancies. Physical Chemistry Chemical Physics, 2011, 13, 923-926.	2.8	17
35	A Comparative Hybrid DFT Study of Phonons in Several SrTiO₃ Phases. Integrated Ferroelectrics, 2011, 123, 18-25.	0.7	4
36	Phonon calculations in cubic and tetragonal phases of SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>: A comparative LCAO and plane-wave study. Physical Review B, 2011, 83, .	3.2	81

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37	Density Functional Theory Calculations On Magnetic Properties Of Actinide Compounds. Materials Research Society Symposia Proceedings, 2011, 1298, 103.	0.1	0
38	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
39	DFT calculations of point defects on UN(001) surface. Surface Science, 2011, 605, 396-400.	1.9	26
40	Helium behavior in oxide nuclear fuels: First principles modeling. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3090-3094.	1.4	30
41	Density functional theory calculations on magnetic properties of actinide compounds. Physical Chemistry Chemical Physics, 2010, 12, 12273.	2.8	58
42	Hybrid density-functional calculations of phonons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaCoO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2010, 82, .	3.2	22
43	Ab initio DFT+U study of He atom incorporation into UO2 crystals. Physical Chemistry Chemical Physics, 2009, 11, 7241.	2.8	72
44	First-principles modelling of radiation defects in advanced nuclear fuels. Nuclear Instruments & Methods in Physics Research B, 2008, 266, 2671-2675.	1.4	14
45	Finite element simulation of diffusion into polycrystalline materials. Solid State Sciences, 2008, 10, 754-760.	3.2	27
46	An improved procedure for determining grain boundary diffusion coefficients from averaged concentration profiles. Journal of Applied Physics, 2008, 103, .	2.5	14
47	Quantitative Model of Electrochemical Ostwald Ripening and Its Application to the Time-Dependent Electrode Potential of Nanocrystalline Metals. Journal of Physical Chemistry B, 2006, 110, 12274-12280.	2.6	35
48	Numerical study of grain boundary diffusion in nanocrystalline ionic materials including blocking space charges. Solid State Ionics, 2006, 177, 1583-1586.	2.7	16
49	Thermodynamic stability and disordering in La Sr1â^'MnO3 solid solutions. Solid State Ionics, 2006, 177, 217-222.	2.7	31
50	Comparative density-functional LCAO and plane-wave calculations ofLaMnO3surfaces. Physical Review B, 2005, 72, .	3.2	84
51	The development of drift-strip detectors based on CdZnTe. IEEE Transactions on Nuclear Science, 2002, 49, 2530-2534.	2.0	8
52	The X-ray response of InP. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2002, 487, 435-440.	1.6	14
53	Technological limitations and processing-generated defects at the development of pixel and strip arrays. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2002, 487, 13-18.	1.6	14
54	The X-ray response of InP: Part B, synchrotron radiation measurements. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2002, 491, 444-451.	1.6	11

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55	Characteristics of InP Î³-Detectors. Instruments and Experimental Techniques, 2001, 44, 462-465.	0.5	1
56	An X-ray Detection Unit Based on GaAs Detector. Instruments and Experimental Techniques, 2000, 43, 815-817.	0.5	1
57	Development of drift-strip detectors based on CdZnTe. , 0, , .		0
58	First Principles Simulations on Surface Properties and Oxidation of Nitride Nuclear Fuels. , 0, , .		5