Oleksandr I Malyi

List of Publications by Year
in descending order

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Version: 2024-02-01

72 papers	3,110 citations	172207 29 h-index	161609 54 g-index
72 all docs	72 docs citations	72 times ranked	4022 citing authors

#	Article	IF	Citations
1	Phosphorene as an anode material for Na-ion batteries: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 13921-13928.	1.3	336
2	Adsorption of metal adatoms on single-layer phosphorene. Physical Chemistry Chemical Physics, 2015, 17, 992-1000.	1.3	280
3	Waterâ€Soluble Sericin Protein Enabling Stable Solidâ€“Electrolyte Interphase for Fast Charging High Voltage Battery Electrode. Advanced Materials, 2017, 29, 1701828.	11.1	147
4	Understanding the Role of Nanostructures for Efficient Hydrogen Generation on Immobilized Photocatalysts. Advanced Energy Materials, 2013, 3, 1368-1380.	10.2	122
5	Ambient dissolutionâ€“recrystallization towards large-scale preparation of V2O5 nanobelts for high-energy battery applications. Nano Energy, 2016, 22, 583-593.	8.2	112
6	In search of high performance anode materials for Mg batteries: Computational studies of Mg in Ge, Si, and Sn. Journal of Power Sources, 2013, 233, 341-345.	4.0	103
7	Direct coherent multi-ink printing of fabric supercapacitors. Science Advances, 2021, 7, .	4.7	95
8	A computational study of Na behavior on graphene. Applied Surface Science, 2015, 333, 235-243.	3.1	90
9	Identifying the Origin and Contribution of Surface Storage in TiO₂(B) Nanotube Electrode by In Situ Dynamic Valence State Monitoring. Advanced Materials, 2018, 30, e1802200.	11.1	90
10	Reducing the Charge Carrier Transport Barrier in Functionally Layerâ€Graded Electrodes. Angewandte Chemie - International Edition, 2017, 56, 14847-14852.	7.2	88
11	A Comparative Computational Study of Structures, Diffusion, and Dopant Interactions between Li and Na Insertion into Si. Applied Physics Express, 2013, 6, 027301.	1.1	87
12	Understanding Doping of Quantum Materials. Chemical Reviews, 2021, 121, 3031-3060.	23.0	86
13	Insertion energetics of lithium, sodium, and magnesium in crystalline and amorphous titanium dioxide: A comparative first-principles study. Journal of Power Sources, 2015, 278, 197-202.	4.0	83
14	A computational study of the insertion of Li, Na, and Mg atoms into Si(111) nanosheets. Nano Energy, 2013, 2, 1149-1157.	8.2	76
15	Energy, Phonon, and Dynamic Stability Criteria of Two-Dimensional Materials. ACS Applied Materials & Interfaces, 2019, 11, 24876-24884.	4.0	76
16	Controlling Na diffusion by rational design of Si-based layered architectures. Physical Chemistry Chemical Physics, 2014, 16, 4260.	1.3	75
17	Comparative computational study of the energetics of Li, Na, and Mg storage in amorphous and crystalline silicon. Computational Materials Science, 2014, 94, 214-217.	1.4	70
18	Enhanced Li adsorption and diffusion in silicon nanosheets based on first principles calculations. RSC Advances, 2013, 3, 4231.	1.7	61

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19	Comparative computational study of the diffusion of Li, Na, and Mg in silicon including the effect of vibrations. Solid State Ionics, 2013, 253, 157-163.	1.3	51
20	Correlating the Peukertâ€™s Constant with Phase Composition of Electrode Materials in Fast Lithiation Processes. , 2019, 1, 519-525.		45
21	Printable Ink Design towards Customizable Miniaturized Energy Storage Devices. , 2020, 2, 1041-1056.		45
22	False metals, real insulators, and degenerate gapped metals. Applied Physics Reviews, 2020, 7, .	5.5	44
23	Deep Cycling for Highâ€Capacity Liâ€Ion Batteries. Advanced Materials, 2021, 33, e2004998.	11.1	43
24	Mechanically Reinforced Localized Structure Design to Stabilize Solidâ€“Electrolyte Interface of the Composited Electrode of Si Nanoparticles and TiO₂ Nanotubes. Small, 2020, 16, e2002094.	5.2	41
25	Formation and migration of oxygen and zirconium vacancies in cubic zirconia and zirconium oxysulfide. Solid State Ionics, 2012, 212, 117-122.	1.3	38
26	Effect of static local distortions vs. dynamic motions on the stability and band gaps of cubic oxide and halide perovskites. Materials Today, 2021, 49, 107-122.	8.3	37
27	Regulating zinc electroplating chemistry to achieve high energy coaxial fiber Zn ion supercapacitor for self-powered textile-based monitoring system. Nano Energy, 2022, 93, 106893.	8.2	36
28	Chemistry of Oxygen Ionosorption on SnO₂ Surfaces. ACS Applied Materials & Interfaces, 2021, 13, 33664-33676.	4.0	35
29	Bulk <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>NdNi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> is thermodynamically unstable with respect to decomposition while hydrogenation reduces the instability and transforms it from metal to insulator. Physical Review B, 2022, 105, .	1.1	33
30	In search of new reconstructions of (001) Î±-quartz surface: a first principles study. RSC Advances, 2014, 4, 55599-55603.	1.7	32
31	Density functional theory study of the effects of alloying additions on sulfur adsorption on nickel surfaces. Applied Surface Science, 2013, 264, 320-328.	3.1	30
32	Stability and electronic properties of phosphorene oxides: from 0-dimensional to amorphous 2-dimensional structures. Nanoscale, 2017, 9, 2428-2435.	2.8	30
33	Realization of predicted exotic materials: The burden of proof. Materials Today, 2020, 32, 35-45.	8.3	29
34	Spontaneous Non-stoichiometry and Ordering in Degenerate but Gapped Transparent Conductors. Matter, 2019, 1, 280-294.	5.0	27
35	Tailoring electronic properties of multilayer phosphorene by siliconization. Physical Chemistry Chemical Physics, 2018, 20, 2075-2083.	1.3	25
36	Mass enhancement in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:r and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>s</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>p</mml:m perovskites from symmetry breaking. Physical Review B, 2021, 103, .	1.1	24

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37	Reducing the Charge Carrier Transport Barrier in Functionally Layerâ€Graded Electrodes. Angewandte Chemie, 2017, 129, 15043-15048.	1.6	23
38	Enhanced Li Adsorption and Diffusion in Singleâ€Walled Silicon Nanotubes: An ab Initio Study. ChemPhysChem, 2013, 14, 1161-1167.	1.0	21
39	Distance-Dependent Sign Reversal in the Casimir-Lifshitz Torque. Physical Review Letters, 2018, 120, 131601.	2.9	21
40	Volume dependence of the dielectric properties of amorphous SiO₂. Physical Chemistry Chemical Physics, 2016, 18, 7483-7489.	1.3	20
41	Comparison of alpha and beta tin for lithium, sodium, and magnesium storage: Anab initiostudy including phonon contributions. Journal of Chemical Physics, 2015, 143, 204701.	1.2	19
42	Amphipathic Molecules Endowing Highly Structure Robust and Fast Kinetic Vanadiumâ€Based Cathode for Highâ€Performance Zincâ€Ion Batteries. Small Structures, 2022, 3, .	6.9	19
43	Density functional theory study of sulfur tolerance of copper: New copperâ€“sulfur phase diagram. Chemical Physics Letters, 2012, 533, 20-24.	1.2	18
44	Effect of sulfur impurity on the stability of cubic zirconia and its interfaces with metals. Journal of Materials Chemistry, 2011, 21, 12363.	6.7	17
45	A first principles study of CO₂ adsorption on Î±-SiO₂(001) surfaces. Physical Chemistry Chemical Physics, 2015, 17, 20125-20133.	1.3	17
46	Band gap modulation of SrTiO₃ upon CO₂ adsorption. Physical Chemistry Chemical Physics, 2017, 19, 16629-16637.	1.3	17
47	First-Principles Mapping of the Electronic Properties of Two-Dimensional Materials for Strain-Tunable Nanoelectronics. ACS Applied Nano Materials, 2019, 2, 5614-5624.	2.4	17
48	Anisotropic contribution to the van der Waals and the Casimir-Polder energies for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>CO</mml:mtext><mml:mn>2</mml:mn></mml:msub> xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>CH</mml:mtext><mml:mn>4</mml:mn></mml:msub> near surfaces and thin films. Physical Review A, 2015, 92, .	1.0	13
49	Suppression of surfaces states at cubic perovskite (001) surfaces by CO2 adsorption. Physical Chemistry Chemical Physics, 2018, 20, 18828-18836.	1.3	13
50	Improved binding and stability in Si/CNT hybrid nanostructures via interfacial functionalization: a first-principles study. RSC Advances, 2013, 3, 8446.	1.7	12
51	Fluid-sensitive nanoscale switching with quantum levitation controlled by <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math> -Sn/ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math> -Sn phase transition. Physical Review B, 2018, 97, .	1.1	12
52	A computational study of the effect of alloying additions on the stability of Ni/c-ZrO2 interfaces. Surface Science, 2013, 611, 5-9.	0.8	11
53	Dispersion Forces Stabilize Ice Coatings at Certain Gas Hydrate Interfaces That Prevent Water Wetting. ACS Earth and Space Chemistry, 2019, 3, 1014-1022.	1.2	11
54	Lifshitz interaction can promote ice growth at water-silica interfaces. Physical Review B, 2017, 95, .	1.1	10

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55	Hole antidoping of oxides. Physical Review B, 2020, 101, .	1.1	10
56	Intrinsic local symmetry breaking in nominally cubic paraelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>BaTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2022, 105, .	1.1	10
57	Noble gas as a functional dopant in ZnO. Npj Computational Materials, 2019, 5, .	3.5	9
58	Local positional and spin symmetry breaking as a source of magnetism and insulation in paramagnetic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>EuTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2022, 6, .	0.9	8
59	A Comparative Computational Study of Li, Na, and Mg Insertion in Î±-Sn. Materials Research Society Symposia Proceedings, 2014, 1678, 1.	0.1	7
60	A comparative computational study of the diffusion of Na and Li atoms in Sn(111) nanosheets. Solid State Ionics, 2014, 268, 273-276.	1.3	7
61	The influence of Lifshitz forces and gas on premelting of ice within porous materials. Europhysics Letters, 2016, 115, 13001.	0.7	7
62	Effects of van der Waals forces and salt ions on the growth of water films on ice and the detachment of CO 2 bubbles. Europhysics Letters, 2016, 113, 43002.	0.7	7
63	Amorphization of Indirect Band Gap Semiconductors To Tune Their Optoelectronic Properties. Journal of Physical Chemistry C, 2020, 124, 14432-14438.	1.5	7
64	Premelting and formation of ice due to Casimir-Lifshitz interactions: Impact of improved parameterization for materials. Physical Review B, 2022, 105, .	1.1	6
65	Dependence of band gaps in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math> -electron perovskite oxides on magnetism. Physical Review B, 2022, 105, .	1.1	6
66	Effect of excess charge carriers and fluid medium on the magnitude and sign of the Casimir-Lifshitz torque. Physical Review B, 2019, 100, .	1.1	4
67	Computational study of Mg insertion into amorphous silicon: advantageous energetics over crystalline silicon for Mg storage. Materials Research Society Symposia Proceedings, 2013, 1540, 3601.	0.1	3
68	Increased porosity turns desorption to adsorption for gas bubbles near water-SiO2interface. Physical Review B, 2015, 91, .	1.1	3
69	Role of Inter-Dopant Interactions on the Diffusion of Li and Na Atoms in Bulk Si Anodes. Materials Research Society Symposia Proceedings, 2013, 1541, 75601.	0.1	2
70	Elementary models of the â€œflux driven anti-ripeningâ€•during nanobelt growth. Physical Chemistry Chemical Physics, 2020, 22, 9740-9748.	1.3	1
71	Siliconâ€Based Anode Materials: Mechanically Reinforced Localized Structure Design to Stabilize Solidâ€“Electrolyte Interface of the Composited Electrode of Si Nanoparticles and TiO₂ Nanotubes (Small 30/2020). Small, 2020, 16, 2070169.	5.2	0
72	Comparative AB Initio Study of Lithium Storage in Amorphous and Crystalline TiO 2. , 2014, , .		0