Oleksandr I Malyi

List of Publications by Year in Descending Order

66 papers	2,202 citations	25 h-index	46 g-index
72 ext. papers	2,650 ext. citations	8.4 avg, IF	5.47 L-index

#	Paper	IF	Citations
66	Bulk NdNiO2 is thermodynamically unstable with respect to decomposition while hydrogenation reduces the instability and transforms it from metal to insulator. *Physical Review B*, **2022**, 105,	3.3	7
65	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	17.1	6
64	Mass enhancement in 3d and sp perovskites from symmetry breaking. *Physical Review B*, **2021**, 103,	3.3	6
63	Understanding Doping of Quantum Materials. *Chemical Reviews*, **2021**, 121, 3031-3060	68.1	27
62	Direct coherent multi-ink printing of fabric supercapacitors. *Science Advances*, **2021**, 7,	14.3	44
61	Deep Cycling for High-Capacity Li-Ion Batteries. *Advanced Materials*, **2021**, 33, e2004998	24	15
60	Chemistry of Oxygen Ionosorption on SnO Surfaces. *ACS Applied Materials & Interfaces*, **2021**, 13, 33664-33676	9.5	9
59	Effect of static local distortions vs. dynamic motions on the stability and band gaps of cubic oxide and halide perovskites. *Materials Today*, **2021**,	21.8	4
58	False metals, real insulators, and degenerate gapped metals. *Applied Physics Reviews*, **2020**, 7, 041310	17.3	15
57	Amorphization of Indirect Band Gap Semiconductors To Tune Their Optoelectronic Properties. *Journal of Physical Chemistry C*, **2020**, 124, 14432-14438	3.8	2
56	Hole antidoping of oxides. *Physical Review B*, **2020**, 101,	3.3	6
55	Mechanically Reinforced Localized Structure Design to Stabilize Solid-Electrolyte Interface of the Composited Electrode of Si Nanoparticles and TiO Nanotubes. *Small*, **2020**, 16, e2002094	11	26
54	Elementary models of the "flux driven anti-ripening" during nanobelt growth. *Physical Chemistry Chemical Physics*, **2020**, 22, 9740-9748	3.6	1
53	Printable Ink Design towards Customizable Miniaturized Energy Storage Devices **2020**, 2, 1041-1056		29
52	Silicon-Based Anode Materials: Mechanically Reinforced Localized Structure Design to Stabilize Solid-Electrolyte Interface of the Composited Electrode of Si Nanoparticles and TiO2 Nanotubes (Small 30/2020). *Small*, **2020**, 16, 2070169	11	
51	Realization of predicted exotic materials: The burden of proof. *Materials Today*, **2020**, 32, 35-45	21.8	17
50	First-Principles Mapping of the Electronic Properties of Two-Dimensional Materials for Strain-Tunable Nanoelectronics. *ACS Applied Nano Materials*, **2019**, 2, 5614-5624	5.6	11

49	Correlating the Peukert Constant with Phase Composition of Electrode Materials in Fast Lithiation Processes **2019**, 1, 519-525		32
48	Dispersion Forces Stabilize Ice Coatings at Certain Gas Hydrate Interfaces That Prevent Water Wetting. *ACS Earth and Space Chemistry*, **2019**, 3, 1014-1022	3.2	7
47	Energy, Phonon, and Dynamic Stability Criteria of Two-Dimensional Materials. *ACS Applied Materials & Interfaces*, **2019**, 11, 24876-24884	9.5	33
46	Noble gas as a functional dopant in ZnO. *Npj Computational Materials*, **2019**, 5,	10.9	3
45	Spontaneous Non-stoichiometry and Ordering in Degenerate but Gapped Transparent Conductors. *Matter*, **2019**, 1, 280-294	12.7	17
44	Effect of excess charge carriers and fluid medium on the magnitude and sign of the Casimir-Lifshitz torque. *Physical Review B*, **2019**, 100,	3.3	1
43	Tailoring electronic properties of multilayer phosphorene by siliconization. *Physical Chemistry Chemical Physics*, **2018**, 20, 2075-2083	3.6	18
42	Distance-Dependent Sign Reversal in the Casimir-Lifshitz Torque. *Physical Review Letters*, **2018**, 120, 131601	7.4	11
41	Fluid-sensitive nanoscale switching with quantum levitation controlled by Sn/Sn phase transition. *Physical Review B*, **2018**, 97,	3.3	7
40	Suppression of surfaces states at cubic perovskite (001) surfaces by CO adsorption. *Physical Chemistry Chemical Physics*, **2018**, 20, 18828-18836	3.6	7
39	Identifying the Origin and Contribution of Surface Storage in TiO (B) Nanotube Electrode by In Situ Dynamic Valence State Monitoring. *Advanced Materials*, **2018**, 30, e1802200	24	72
38	Stability and electronic properties of phosphorene oxides: from 0-dimensional to amorphous 2-dimensional structures. *Nanoscale*, **2017**, 9, 2428-2435	7.7	26
37	Band gap modulation of SrTiO upon CO adsorption. *Physical Chemistry Chemical Physics*, **2017**, 19, 16629-16637	3.6	14
36	Reducing the Charge Carrier Transport Barrier in Functionally Layer-Graded Electrodes. *Angewandte Chemie*, **2017**, 129, 15043-15048	3.6	15
35	Reducing the Charge Carrier Transport Barrier in Functionally Layer-Graded Electrodes. *Angewandte Chemie - International Edition*, **2017**, 56, 14847-14852	16.4	71
34	Lifshitz interaction can promote ice growth at water-silica interfaces. *Physical Review B*, **2017**, 95,	3.3	6
33	Water-Soluble Sericin Protein Enabling Stable Solid-Electrolyte Interphase for Fast Charging High Voltage Battery Electrode. *Advanced Materials*, **2017**, 29, 1701828	24	114
32	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	1.6	6

31	Volume dependence of the dielectric properties of amorphous SiO2. *Physical Chemistry Chemical Physics*, **2016**, 18, 7483-9	3.6	13
30	Ambient dissolution□ecrystallization towards large-scale preparation of V 2 O 5 nanobelts for high-energy battery applications. *Nano Energy*, **2016**, 22, 583-593	17.1	82
29	The influence of Lifshitz forces and gas on premelting of ice within porous materials. *Europhysics Letters*, **2016**, 115, 13001	1.6	5
28	A first principles study of CO2 adsorption on □SiO2(001) surfaces. *Physical Chemistry Chemical Physics*, **2015**, 17, 20125-33	3.6	13
27	Phosphorene as an anode material for Na-ion batteries: a first-principles study. *Physical Chemistry Chemical Physics*, **2015**, 17, 13921-8	3.6	267
26	Adsorption of metal adatoms on single-layer phosphorene. *Physical Chemistry Chemical Physics*, **2015**, 17, 992-1000	3.6	246
25	Anisotropic contribution to the van der Waals and the Casimir-Polder energies for CO2 and CH4 molecules near surfaces and thin films. *Physical Review A*, **2015**, 92,	2.6	9
24	Increased porosity turns desorption to adsorption for gas bubbles near water-SiO2 interface. *Physical Review B*, **2015**, 91,	3.3	3
23	Comparison of alpha and beta tin for lithium, sodium, and magnesium storage: An ab initio study including phonon contributions. *Journal of Chemical Physics*, **2015**, 143, 204701	3.9	15
22	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	8.9	69
21	A computational study of Na behavior on graphene. *Applied Surface Science*, **2015**, 333, 235-243	6.7	71
20	Controlling Na diffusion by rational design of Si-based layered architectures. *Physical Chemistry Chemical Physics*, **2014**, 16, 4260-7	3.6	62
19	A comparative computational study of the diffusion of Na and Li atoms in Sn(111) nanosheets. *Solid State Ionics*, **2014**, 268, 273-276	3.3	5
18	Comparative computational study of the energetics of Li, Na, and Mg storage in amorphous and crystalline silicon. *Computational Materials Science*, **2014**, 94, 214-217	3.2	56
17	In search of new reconstructions of (001) □quartz surface: a first principles study. *RSC Advances*, **2014**, 4, 55599-55603	3.7	22
16	A Comparative Computational Study of Li, Na, and Mg Insertion in □Sn. *Materials Research Society Symposia Proceedings*, **2014**, 1678, 1		7
15	A computational study of the effect of alloying additions on the stability of Ni/c-ZrO2 interfaces. *Surface Science*, **2013**, 611, 5-9	1.8	10
14	A computational study of the insertion of Li, Na, and Mg atoms into Si(111) nanosheets. *Nano Energy*, **2013**, 2, 1149-1157	17.1	68

13	A Comparative Computational Study of Structures, Diffusion, and Dopant Interactions between Li and Na Insertion into Si. *Applied Physics Express*, **2013**, 6, 027301	2.4	71
12	Improved binding and stability in Si/CNT hybrid nanostructures via interfacial functionalization: a first-principles study. *RSC Advances*, **2013**, 3, 8446	3.7	11
11	Density functional theory study of the effects of alloying additions on sulfur adsorption on nickel surfaces. *Applied Surface Science*, **2013**, 264, 320-328	6.7	25
10	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	3.3	43
9	Enhanced Li adsorption and diffusion in silicon nanosheets based on first principles calculations. *RSC Advances*, **2013**, 3, 4231	3.7	48
8	Enhanced Li adsorption and diffusion in single-walled silicon nanotubes: an ab initio study. *ChemPhysChem*, **2013**, 14, 1161-7	3.2	21
7	Understanding the Role of Nanostructures for Efficient Hydrogen Generation on Immobilized Photocatalysts. *Advanced Energy Materials*, **2013**, 3, 1368-1380	21.8	118
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	8.9	85
5	Computational study of Mg insertion into amorphous silicon: advantageous energetics over crystalline silicon for Mg storage. *Materials Research Society Symposia Proceedings*, **2013**, 1540, 3601		3
4	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		2
3	Density functional theory study of sulfur tolerance of copper: New copper–sulfur phase diagram. *Chemical Physics Letters*, **2012**, 533, 20-24	2.5	17
2	Formation and migration of oxygen and zirconium vacancies in cubic zirconia and zirconium oxysulfide. *Solid State Ionics*, **2012**, 212, 117-122	3.3	35
1	Effect of sulfur impurity on the stability of cubic zirconia and its interfaces with metals. *Journal of Materials Chemistry*, **2011**, 21, 12363		13