

# Oleksandr I Malyi

## List of Publications by Citations

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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	Phosphorene as an anode material for Na-ion batteries: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 13921-8	3.6	267
65	Adsorption of metal adatoms on single-layer phosphorene. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 992-1000	3.6	246
64	Understanding the Role of Nanostructures for Efficient Hydrogen Generation on Immobilized Photocatalysts. <i>Advanced Energy Materials</i> , <b>2013</b> , 3, 1368-1380	21.8	118
63	Water-Soluble Sericin Protein Enabling Stable Solid-Electrolyte Interphase for Fast Charging High Voltage Battery Electrode. <i>Advanced Materials</i> , <b>2017</b> , 29, 1701828	24	114
62	In search of high performance anode materials for Mg batteries: Computational studies of Mg in Ge, Si, and Sn. <i>Journal of Power Sources</i> , <b>2013</b> , 233, 341-345	8.9	85
61	Ambient dissolution/recrystallization towards large-scale preparation of V <sub>2</sub> O <sub>5</sub> nanobelts for high-energy battery applications. <i>Nano Energy</i> , <b>2016</b> , 22, 583-593	17.1	82
60	Identifying the Origin and Contribution of Surface Storage in TiO <sub>2</sub> (B) Nanotube Electrode by In Situ Dynamic Valence State Monitoring. <i>Advanced Materials</i> , <b>2018</b> , 30, e1802200	24	72
59	Reducing the Charge Carrier Transport Barrier in Functionally Layer-Graded Electrodes. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 14847-14852	16.4	71
58	A Comparative Computational Study of Structures, Diffusion, and Dopant Interactions between Li and Na Insertion into Si. <i>Applied Physics Express</i> , <b>2013</b> , 6, 027301	2.4	71
57	A computational study of Na behavior on graphene. <i>Applied Surface Science</i> , <b>2015</b> , 333, 235-243	6.7	71
56	Insertion energetics of lithium, sodium, and magnesium in crystalline and amorphous titanium dioxide: A comparative first-principles study. <i>Journal of Power Sources</i> , <b>2015</b> , 278, 197-202	8.9	69
55	A computational study of the insertion of Li, Na, and Mg atoms into Si(111) nanosheets. <i>Nano Energy</i> , <b>2013</b> , 2, 1149-1157	17.1	68
54	Controlling Na diffusion by rational design of Si-based layered architectures. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 4260-7	3.6	62
53	Comparative computational study of the energetics of Li, Na, and Mg storage in amorphous and crystalline silicon. <i>Computational Materials Science</i> , <b>2014</b> , 94, 214-217	3.2	56
52	Enhanced Li adsorption and diffusion in silicon nanosheets based on first principles calculations. <i>RSC Advances</i> , <b>2013</b> , 3, 4231	3.7	48
51	Direct coherent multi-ink printing of fabric supercapacitors. <i>Science Advances</i> , <b>2021</b> , 7,	14.3	44
50	Comparative computational study of the diffusion of Li, Na, and Mg in silicon including the effect of vibrations. <i>Solid State Ionics</i> , <b>2013</b> , 253, 157-163	3.3	43

49	Formation and migration of oxygen and zirconium vacancies in cubic zirconia and zirconium oxysulfide. <i>Solid State Ionics</i> , <b>2012</b> , 212, 117-122	3.3	35
48	Energy, Phonon, and Dynamic Stability Criteria of Two-Dimensional Materials. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 24876-24884	9.5	33
47	Correlating the Peukert's Constant with Phase Composition of Electrode Materials in Fast Lithiation Processes <b>2019</b> , 1, 519-525		32
46	Printable Ink Design towards Customizable Miniaturized Energy Storage Devices <b>2020</b> , 2, 1041-1056		29
45	Understanding Doping of Quantum Materials. <i>Chemical Reviews</i> , <b>2021</b> , 121, 3031-3060	68.1	27
44	Stability and electronic properties of phosphorene oxides: from 0-dimensional to amorphous 2-dimensional structures. <i>Nanoscale</i> , <b>2017</b> , 9, 2428-2435	7.7	26
43	Mechanically Reinforced Localized Structure Design to Stabilize Solid-Electrolyte Interface of the Compositated Electrode of Si Nanoparticles and TiO Nanotubes. <i>Small</i> , <b>2020</b> , 16, e2002094	11	26
42	Density functional theory study of the effects of alloying additions on sulfur adsorption on nickel surfaces. <i>Applied Surface Science</i> , <b>2013</b> , 264, 320-328	6.7	25
41	In search of new reconstructions of (001) $\beta$ -quartz surface: a first principles study. <i>RSC Advances</i> , <b>2014</b> , 4, 55599-55603	3.7	22
40	Enhanced Li adsorption and diffusion in single-walled silicon nanotubes: an ab initio study. <i>ChemPhysChem</i> , <b>2013</b> , 14, 1161-7	3.2	21
39	Tailoring electronic properties of multilayer phosphorene by siliconization. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 2075-2083	3.6	18
38	Spontaneous Non-stoichiometry and Ordering in Degenerate but Gapped Transparent Conductors. <i>Matter</i> , <b>2019</b> , 1, 280-294	12.7	17
37	Density functional theory study of sulfur tolerance of copper: New copper-sulfur phase diagram. <i>Chemical Physics Letters</i> , <b>2012</b> , 533, 20-24	2.5	17
36	Realization of predicted exotic materials: The burden of proof. <i>Materials Today</i> , <b>2020</b> , 32, 35-45	21.8	17
35	Reducing the Charge Carrier Transport Barrier in Functionally Layer-Graded Electrodes. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 15043-15048	3.6	15
34	False metals, real insulators, and degenerate gapped metals. <i>Applied Physics Reviews</i> , <b>2020</b> , 7, 041310	17.3	15
33	Comparison of alpha and beta tin for lithium, sodium, and magnesium storage: An ab initio study including phonon contributions. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 204701	3.9	15
32	Deep Cycling for High-Capacity Li-Ion Batteries. <i>Advanced Materials</i> , <b>2021</b> , 33, e2004998	24	15

31	Band gap modulation of SrTiO upon CO adsorption. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 16629-16637	3.6	14
30	A first principles study of CO <sub>2</sub> adsorption on SiO <sub>2</sub> (001) surfaces. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 20125-33	3.6	13
29	Volume dependence of the dielectric properties of amorphous SiO <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 7483-9	3.6	13
28	Effect of sulfur impurity on the stability of cubic zirconia and its interfaces with metals. <i>Journal of Materials Chemistry</i> , <b>2011</b> , 21, 12363		13
27	First-Principles Mapping of the Electronic Properties of Two-Dimensional Materials for Strain-Tunable Nanoelectronics. <i>ACS Applied Nano Materials</i> , <b>2019</b> , 2, 5614-5624	5.6	11
26	Distance-Dependent Sign Reversal in the Casimir-Lifshitz Torque. <i>Physical Review Letters</i> , <b>2018</b> , 120, 131601	7.4	11
25	Improved binding and stability in Si/CNT hybrid nanostructures via interfacial functionalization: a first-principles study. <i>RSC Advances</i> , <b>2013</b> , 3, 8446	3.7	11
24	A computational study of the effect of alloying additions on the stability of Ni/c-ZrO <sub>2</sub> interfaces. <i>Surface Science</i> , <b>2013</b> , 611, 5-9	1.8	10
23	Anisotropic contribution to the van der Waals and the Casimir-Polder energies for CO <sub>2</sub> and CH <sub>4</sub> molecules near surfaces and thin films. <i>Physical Review A</i> , <b>2015</b> , 92,	2.6	9
22	Chemistry of Oxygen Ion Adsorption on SnO Surfaces. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 33664-33676	9.5	9
21	Dispersion Forces Stabilize Ice Coatings at Certain Gas Hydrate Interfaces That Prevent Water Wetting. <i>ACS Earth and Space Chemistry</i> , <b>2019</b> , 3, 1014-1022	3.2	7
20	Fluid-sensitive nanoscale switching with quantum levitation controlled by $\mathbb{F}_n/\mathbb{F}_n$ phase transition. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	7
19	Suppression of surface states at cubic perovskite (001) surfaces by CO adsorption. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 18828-18836	3.6	7
18	A Comparative Computational Study of Li, Na, and Mg Insertion in $\mathbb{F}_n$ . <i>Materials Research Society Symposia Proceedings</i> , <b>2014</b> , 1678, 1		7
17	Bulk NdNiO <sub>2</sub> is thermodynamically unstable with respect to decomposition while hydrogenation reduces the instability and transforms it from metal to insulator. <i>Physical Review B</i> , <b>2022</b> , 105,	3.3	7
16	Hole antidoping of oxides. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	6
15	Effects of van der Waals forces and salt ions on the growth of water films on ice and the detachment of CO <sub>2</sub> bubbles. <i>Europhysics Letters</i> , <b>2016</b> , 113, 43002	1.6	6
14	Lifshitz interaction can promote ice growth at water-silica interfaces. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	6

13	Regulating zinc electroplating chemistry to achieve high energy coaxial fiber Zn ion supercapacitor for self-powered textile-based monitoring system. <i>Nano Energy</i> , <b>2022</b> , 93, 106893	17.1	6
12	Mass enhancement in 3d and s $\bar{p}$ perovskites from symmetry breaking. <i>Physical Review B</i> , <b>2021</b> , 103,	3.3	6
11	A comparative computational study of the diffusion of Na and Li atoms in Sn(111) nanosheets. <i>Solid State Ionics</i> , <b>2014</b> , 268, 273-276	3.3	5
10	The influence of Lifshitz forces and gas on premelting of ice within porous materials. <i>Europhysics Letters</i> , <b>2016</b> , 115, 13001	1.6	5
9	Effect of static local distortions vs. dynamic motions on the stability and band gaps of cubic oxide and halide perovskites. <i>Materials Today</i> , <b>2021</b> ,	21.8	4
8	Noble gas as a functional dopant in ZnO. <i>Npj Computational Materials</i> , <b>2019</b> , 5,	10.9	3
7	Increased porosity turns desorption to adsorption for gas bubbles near water-SiO <sub>2</sub> interface. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	3
6	Computational study of Mg insertion into amorphous silicon: advantageous energetics over crystalline silicon for Mg storage. <i>Materials Research Society Symposia Proceedings</i> , <b>2013</b> , 1540, 3601		3
5	Amorphization of Indirect Band Gap Semiconductors To Tune Their Optoelectronic Properties. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 14432-14438	3.8	2
4	Role of Inter-Dopant Interactions on the Diffusion of Li and Na Atoms in Bulk Si Anodes. <i>Materials Research Society Symposia Proceedings</i> , <b>2013</b> , 1541, 75601		2
3	Elementary models of the "flux driven anti-ripening" during nanobelt growth. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 9740-9748	3.6	1
2	Effect of excess charge carriers and fluid medium on the magnitude and sign of the Casimir-Lifshitz torque. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	1
1	Silicon-Based Anode Materials: Mechanically Reinforced Localized Structure Design to Stabilize Solid Electrolyte Interface of the Composited Electrode of Si Nanoparticles and TiO <sub>2</sub> Nanotubes (Small 30/2020). <i>Small</i> , <b>2020</b> , 16, 2070169	11	