

Mohammad Khazaei

List of Publications by Year in descending order

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54
papers

5,147
citations

279701

23
h-index

197736

49
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all docs

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docs citations

54
times ranked

4759
citing authors

#	ARTICLE	IF	CITATIONS
1	Novel Electronic and Magnetic Properties of Two-Dimensional Transition Metal Carbides and Nitrides. <i>Advanced Functional Materials</i> , 2013, 23, 2185-2192.	7.8	1,418
2	Electronic properties and applications of MXenes: a theoretical review. <i>Journal of Materials Chemistry C</i> , 2017, 5, 2488-2503.	2.7	759
3	Two-dimensional molybdenum carbides: potential thermoelectric materials of the MXene family. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7841-7849.	1.3	395
4	OH-terminated two-dimensional transition metal carbides and nitrides as ultralow work function materials. <i>Physical Review B</i> , 2015, 92, .	1.1	342
5	Recent advances in MXenes: From fundamentals to applications. <i>Current Opinion in Solid State and Materials Science</i> , 2019, 23, 164-178.	5.6	247
6	Large-gap two-dimensional topological insulator in oxygen functionalized MXene. <i>Physical Review B</i> , 2015, 92, .	1.1	229
7	Topological insulators in the ordered double transition metals M_2C_2 MXenes		

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19	Chemical engineering of prehydrogenated C and BN-sheets by Li: Application in hydrogen storage. <i>Journal of Applied Physics</i> , 2009, 106, .	1.1	40
20	Electronic and magnetic properties of carbide MXenes—the role of electron correlations. <i>Materials Today Advances</i> , 2021, 9, 100118.	2.5	35
21	Discovery of stable and intrinsic antiferromagnetic iron oxyhalide monolayers. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11731-11739.	1.3	32
22	Electronic structures of iMAX phases and their two-dimensional derivatives: A family of piezoelectric materials. <i>Physical Review Materials</i> , 2018, 2, .	0.9	31
23	Geometrical indications of adsorbed hydrogen atoms on graphite producing star and ellipsoidal like features in scanning tunneling microscopy images: Ab initio study. <i>Carbon</i> , 2009, 47, 3306-3312.	5.4	26
24	Computational Design of a Rectifying Diode Made by Interconnecting Carbon Nanotubes with Peptide Linkages. <i>Journal of Physical Chemistry C</i> , 2007, 111, 12175-12180.	1.5	24
25	Field Emission Signature of Pentagons at Carbon Nanotube Caps. <i>Journal of Physical Chemistry C</i> , 2007, 111, 6690-6693.	1.5	24
26	Dynamical Criteria for Cs Ion Insertion and Adsorption at Cap and Stem of Carbon Nanotubes: Ab Initio Study and Comparison with Experiment. <i>Journal of Physical Chemistry B</i> , 2004, 108, 15529-15535.	1.2	21
27	Modulation of nearly free electron states in hydroxyl-functionalized MXenes: a first-principles study. <i>Journal of Materials Chemistry C</i> , 2020, 8, 5211-5221.	2.7	21
28	Designing Nanogadgets by Interconnecting Carbon Nanotubes with Zinc Layers. <i>ACS Nano</i> , 2008, 2, 939-943.	7.3	20
29	Exploring structural, electronic, and mechanical properties of 2D hexagonal MBenes. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 155503.	0.7	20
30	Effects of Alkali Adatoms on CO and H ₂ S Adsorptions on the Fe(100) Surface: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23893-23901.	1.5	19
31	Hypercoordinate two-dimensional transition-metal borides for spintronics and catalyst applications. <i>Journal of Materials Chemistry C</i> , 0, , .	2.7	18
32	Chemical engineering of adamantane by lithium functionalization: A first-principles density functional theory study. <i>Physical Review B</i> , 2011, 83, .	1.1	17
33	Electron transport through carbon nanotube intramolecular heterojunctions with peptide linkages. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5225.	1.3	16
34	First-principles simulation of cyanogen under high pressure: Formation of paracyanogen and an insulating carbon nitride solid. <i>Physical Review B</i> , 2011, 83, .	1.1	16
35	Effects of Cs treatment on field emission properties of capped carbon nanotubes. <i>Surface Science</i> , 2007, 601, 1501-1506.	0.8	14
36	Mechanically reliable thermoelectric (TE) nanocomposites by dispersing and embedding TE-nanostructures inside a tetragonal ZrO ₂ matrix: the concept and experimental demonstration in graphene oxide—3YSZ system. <i>Science and Technology of Advanced Materials</i> , 2014, 15, 014201.	2.8	14

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37	Evolutionary structure prediction of two-dimensional IrB ₁₄ : a promising gas sensor material. <i>Journal of Materials Chemistry C</i> , 2018, 6, 5803-5811.	2.7	13
38	MXene Phase with C ₃ Structure Unit: A Family of 2D Electrides. <i>Advanced Functional Materials</i> , 2021, 31, 2100009.	7.8	13
39	High-pressure phases of hydrogen cyanide: formation of hydrogenated carbon nitride polymers and layers and their electronic properties. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 405403.	0.7	11
40	Polymerization of Tetracyanoethylene under Pressure. <i>Journal of Physical Chemistry C</i> , 2013, 117, 712-720.	1.5	10
41	Cs doping effects on electronic structure of thin nanotubes. <i>Computational Materials Science</i> , 2006, 36, 152-158.	1.4	8
42	Quantum-Chemical Design of Covalent Linkages for Interconnecting Carbon Nanotubes. <i>Materials Transactions</i> , 2007, 48, 2148-2151.	0.4	6
43	Electronic Properties and Applications of MXenes from Ab Initio Calculations Perspective. , 2019, , 255-289.		6
44	First-principles study of a topological phase transition induced by image potential states in MXenes. <i>Physical Review B</i> , 2021, 103, .	1.1	6
45	Facile Synthesis of Ti ₂ AC (A = Zn, Al, In, and Ga) MAX Phases by Hydrogen Incorporation into Crystallographic Voids. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11245-11251.	2.1	6
46	Polymerization of cyanoacetylene under pressure: Formation of carbon nitride polymers and bulk structures. <i>Physical Review B</i> , 2012, 85, .	1.1	5
47	An ab initio study of single-walled nanotubes bombarded with 50–150 eV Cs ⁺ ions. <i>Chemical Physics Letters</i> , 2005, 415, 34-39.	1.2	4
48	Considering the effect of different arrangements of pentagons on density of states of capped carbon nanotubes. <i>Physica B: Condensed Matter</i> , 2011, 406, 3885-3890.	1.3	4
49	Phase diagram exploration of TcAlB to two-dimensional Tc ₂ B ₂ . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22086-22095.	1.3	3
50	Electronic Structures of Group III–V Element Haeckelite Compounds: A Novel Family of Semiconductors, Dirac Semimetals, and Topological Insulators. <i>Advanced Functional Materials</i> , 0, , 2110930.	7.8	3
51	Carbon Nanotubes Oscillation under Electric Field. <i>Japanese Journal of Applied Physics</i> , 2010, 49, 115103.	0.8	2
52	Symmetry Rule of the Landau Free Energy in the Phonon-Originating Phase Transition. <i>Journal of the Physical Society of Japan</i> , 2013, 82, 084601.	0.7	1
53	Strain Engineering to Release Trapped Hole Carriers in p-Type Haeckelite GaN. <i>ACS Applied Electronic Materials</i> , 2021, 3, 5257-5264.	2.0	1
54	2D Electrides: MXene Phase with C ₃ Structure Unit: A Family of 2D Electrides (Adv. Funct.)	7.8	10