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 g-index
54 all docs	54 docs citations	54 times ranked	4759 citing authors

#	Article	IF	Citations
1	Electronic and magnetic properties of carbide MXenesâ€"the role of electron correlations. Materials Today Advances, 2021, 9, 100118.	2.5	35
2	First-principles study of a topological phase transition induced by image potential states in MXenes. Physical Review B, 2021, 103, .	1.1	6
3	Exploring structural, electronic, and mechanical properties of 2D hexagonal MBenes. Journal of Physics Condensed Matter, 2021, 33, 155503.	0.7	20
4	MXene Phase with C₃ Structure Unit: A Family of 2D Electrides. Advanced Functional Materials, 2021, 31, 2100009.	7.8	13
5	2D Electrides: MXene Phase with C₃ Structure Unit: A Family of 2D Electrides (Adv. Funct.) Tj ETQq1 1 0.784314 rgBT /Ove	7.8	0
6	Phase diagram exploration of Tcâ€"Alâ€"B: from bulk Tc₂AlB₂ to two-dimensional Tc₂B₂. Physical Chemistry Chemical Physics, 2021, 23, 22086-22095.	1.3	3
7	High-throughput computational discovery of ternary-layered MAX phases and prediction of their exfoliation for formation of 2D MXenes. Nanoscale, 2021, 13, 7294-7307.	2.8	59
8	Strain Engineering to Release Trapped Hole Carriers in p-Type Haeckelite GaN. ACS Applied Electronic Materials, 2021, 3, 5257-5264.	2.0	1
9	Facile Synthesis of Ti₂AC (A = Zn, Al, In, and Ga) MAX Phases by Hydrogen Incorporation into Crystallographic Voids. Journal of Physical Chemistry Letters, 2021, 12, 11245-11251.	2.1	6
10	Modulation of nearly free electron states in hydroxyl-functionalized MXenes: a first-principles study. Journal of Materials Chemistry C, 2020, 8, 5211-5221.	2.7	21
11	Discovery of stable and intrinsic antiferromagnetic iron oxyhalide monolayers. Physical Chemistry Chemical Physics, 2020, 22, 11731-11739.	1.3	32
12	Electronic Properties and Applications of MXenes from Ab Initio Calculations Perspective. , 2019, , 255-289.		6
13	Recent advances in MXenes: From fundamentals to applications. Current Opinion in Solid State and Materials Science, 2019, 23, 164-178.	5.6	247
14	Novel MAB phases and insights into their exfoliation into 2D MBenes. Nanoscale, 2019, 11, 11305-11314.	2.8	120
15	Insights into exfoliation possibility of MAX phases to MXenes. Physical Chemistry Chemical Physics, 2018, 20, 8579-8592.	1.3	182
16	Evolutionary structure prediction of two-dimensional IrB₁₄: a promising gas sensor material. Journal of Materials Chemistry C, 2018, 6, 5803-5811.	2.7	13
17	Electronic structures of iMAX phases and their two-dimensional derivatives: A family of piezoelectric materials. Physical Review Materials, 2018, 2, .	0.9	31
18	Electronic properties and applications of MXenes: a theoretical review. Journal of Materials Chemistry C, 2017, 5, 2488-2503.	2.7	759

#	Article	IF	Citations
19	Theoretical prediction of two-dimensional functionalized MXene nitrides as topological insulators. Physical Review B, 2017, 96, .	1.1	83
20	Semimetallic Two-Dimensional TiB₁₂: Improved Stability and Electronic Properties Tunable by Biaxial Strain. Chemistry of Materials, 2017, 29, 5922-5930.	3.2	41
21	Topological insulators in the ordered double transition metals<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msubsup><mml:mi>M</mml:mi><mml:mn>2</mml:mn><mml:mn mathvariant="normal">C</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>MXenes		

#	Article	IF	Citations
37	Chemical engineering of adamantane by lithium functionalization: A first-principles density functional theory study. Physical Review B, 2011, 83, .	1.1	17
38	Carbon Nanotubes Oscillation under Electric Field. Japanese Journal of Applied Physics, 2010, 49, 115103.	0.8	2
39	First-principles study of structural stability, magnetism, and hyperfine coupling in hydrogen clusters adsorbed on graphene. Physical Review B, 2010, 82, .	1.1	44
40	First-principles study of hydrogen storage over Ni and Rh doped BN sheets. Chemical Physics, 2009, 359, 173-178.	0.9	84
41	Geometrical indications of adsorbed hydrogen atoms on graphite producing star and ellipsoidal like features in scanning tunneling microscopy images: Ab initio study. Carbon, 2009, 47, 3306-3312.	5.4	26
42	Chemical engineering of prehydrogenated C and BN-sheets by Li: Application in hydrogen storage. Journal of Applied Physics, 2009, 106, .	1.1	40
43	Electron transport through carbon nanotube intramolecular heterojunctions with peptide linkages. Physical Chemistry Chemical Physics, 2008, 10, 5225.	1.3	16
44	Designing Nanogadgets by Interconnecting Carbon Nanotubes with Zinc Layers. ACS Nano, 2008, 2, 939-943.	7.3	20
45	Quantum-Chemical Design of Covalent Linkages for Interconnecting Carbon Nanotubes. Materials Transactions, 2007, 48, 2148-2151.	0.4	6
46	Computational Design of a Rectifying Diode Made by Interconnecting Carbon Nanotubes with Peptide Linkages. Journal of Physical Chemistry C, 2007, 111, 12175-12180.	1.5	24
47	Field Emission Signature of Pentagons at Carbon Nanotube Caps. Journal of Physical Chemistry C, 2007, 111, 6690-6693.	1.5	24
48	Effects of Cs treatment on field emission properties of capped carbon nanotubes. Surface Science, 2007, 601, 1501-1506.	0.8	14
49	Cs doping effects on electronic structure of thin nanotubes. Computational Materials Science, 2006, 36, 152-158.	1.4	8
50	An ab initio study of single-walled nanotubes bombarded with 50â€“150eV Cs+ ions. Chemical Physics Letters, 2005, 415, 34-39.	1.2	4
51	Field Emission Patterns from First-Principles Electronic Structures: Application to Pristine and Cesium-Doped Carbon Nanotubes. Physical Review Letters, 2005, 95, 177602.	2.9	48
52	Dynamical Criteria for Cs Ion Insertion and Adsorption at Cap and Stem of Carbon Nanotubes:Â Ab Initio Study and Comparison with Experiment. Journal of Physical Chemistry B, 2004, 108, 15529-15535.	1.2	21
53	Hypercoordinate two-dimensional transition-metal borides for spintronics and catalyst applications. Journal of Materials Chemistry C, 0, , .	2.7	18
54	Electronic Structures of Group IIIâ€“V Element Haeckelite Compounds: A Novel Family of Semiconductors, Dirac Semimetals, and Topological Insulators. Advanced Functional Materials, 0, , 2110930.	7.8	3