## Mohammad Khazaei

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Novel Electronic and Magnetic Properties of Twoâ€Dimensional Transition Metal Carbides and Nitrides. Advanced Functional Materials, 2013, 23, 2185-2192.	14.9	1,418
2	Electronic properties and applications of MXenes: a theoretical review. Journal of Materials Chemistry C, 2017, 5, 2488-2503.	5.5	759
3	Two-dimensional molybdenum carbides: potential thermoelectric materials of the MXene family. Physical Chemistry Chemical Physics, 2014, 16, 7841-7849.	2.8	395
4	OH-terminated two-dimensional transition metal carbides and nitrides as ultralow work function materials. Physical Review B, 2015, 92, .	3.2	342
5	Recent advances in MXenes: From fundamentals to applications. Current Opinion in Solid State and Materials Science, 2019, 23, 164-178.	11.5	247
6	Large-gap two-dimensional topological insulator in oxygen functionalized MXene. Physical Review B, 2015, 92, .	3.2	229
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19	Chemical engineering of prehydrogenated C and BN-sheets by Li: Application in hydrogen storage. Journal of Applied Physics, 2009, 106, .	2.5	40
20	Electronic and magnetic properties of carbide MXenes—the role of electron correlations. Materials Today Advances, 2021, 9, 100118.	5.2	35
21	Discovery of stable and intrinsic antiferromagnetic iron oxyhalide monolayers. Physical Chemistry Chemical Physics, 2020, 22, 11731-11739.	2.8	32
22	Electronic structures of iMAX phases and their two-dimensional derivatives: A family of piezoelectric materials. Physical Review Materials, 2018, 2, .	2.4	31
23	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.	10.3	26
24	Computational Design of a Rectifying Diode Made by Interconnecting Carbon Nanotubes with Peptide Linkages. Journal of Physical Chemistry C, 2007, 111, 12175-12180.	3.1	24
25	Field Emission Signature of Pentagons at Carbon Nanotube Caps. Journal of Physical Chemistry C, 2007, 111, 6690-6693.	3.1	24
26	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.	2.6	21
27	Modulation of nearly free electron states in hydroxyl-functionalized MXenes: a first-principles study. Journal of Materials Chemistry C, 2020, 8, 5211-5221.	5.5	21
28	Designing Nanogadgets by Interconnecting Carbon Nanotubes with Zinc Layers. ACS Nano, 2008, 2, 939-943.	14.6	20
29	Exploring structural, electronic, and mechanical properties of 2D hexagonal MBenes. Journal of Physics Condensed Matter, 2021, 33, 155503.	1.8	20
30	Effects of Alkali Adatoms on CO and H <sub>2</sub> S Adsorptions on the Fe(100) Surface: A Density Functional Theory Study. Journal of Physical Chemistry C, 2011, 115, 23893-23901.	3.1	19
31	Hypercoordinate two-dimensional transition-metal borides for spintronics and catalyst applications. Journal of Materials Chemistry C, 0, , .	5.5	18
32	Chemical engineering of adamantane by lithium functionalization: A first-principles density functional theory study. Physical Review B, 2011, 83, .	3.2	17
33	Electron transport through carbon nanotube intramolecular heterojunctions with peptide linkages. Physical Chemistry Chemical Physics, 2008, 10, 5225.	2.8	16
34	First-principles simulation of cyanogen under high pressure: Formation of paracyanogen and an insulating carbon nitride solid. Physical Review B, 2011, 83, .	3.2	16
35	Effects of Cs treatment on field emission properties of capped carbon nanotubes. Surface Science, 2007, 601, 1501-1506.	1.9	14
36	Mechanically reliable thermoelectric (TE) nanocomposites by dispersing and embedding TE-nanostructures inside a tetragonal ZrO2matrix: the concept and experimental demonstration in graphene oxide–3YSZ system. Science and Technology of Advanced Materials, 2014, 15, 014201.	6.1	14

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37	Evolutionary structure prediction of two-dimensional IrB <sub>14</sub> : a promising gas sensor material. Journal of Materials Chemistry C, 2018, 6, 5803-5811.	5.5	13
38	MXene Phase with C <sub>3</sub> Structure Unit: A Family of 2D Electrides. Advanced Functional Materials, 2021, 31, 2100009.	14.9	13
39	High-pressure phases of hydrogen cyanide: formation of hydrogenated carbon nitride polymers and layers and their electronic properties. Journal of Physics Condensed Matter, 2011, 23, 405403.	1.8	11
40	Polymerization of Tetracyanoethylene under Pressure. Journal of Physical Chemistry C, 2013, 117, 712-720.	3.1	10
41	Cs doping effects on electronic structure of thin nanotubes. Computational Materials Science, 2006, 36, 152-158.	3.0	8
42	Quantum-Chemical Design of Covalent Linkages for Interconnecting Carbon Nanotubes. Materials Transactions, 2007, 48, 2148-2151.	1.2	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. Physical Review B, 2021, 103, .	3.2	6
45	Facile Synthesis of Ti <sub>2</sub> AC (A = Zn, Al, In, and Ga) MAX Phases by Hydrogen Incorporation into Crystallographic Voids. Journal of Physical Chemistry Letters, 2021, 12, 11245-11251.	4.6	6
46	Polymerization of cyanoacetylene under pressure: Formation of carbon nitride polymers and bulk structures. Physical Review B, 2012, 85, .	3.2	5
47	An ab initio study of single-walled nanotubes bombarded with 50–150eV Cs+ ions. Chemical Physics Letters, 2005, 415, 34-39.	2.6	4
48	Considering the effect of different arrangements of pentagons on density of states of capped carbon nanotubes. Physica B: Condensed Matter, 2011, 406, 3885-3890.	2.7	4
49	Phase diagram exploration of Tc–Al–B: from bulk Tc <sub>2</sub> AlB <sub>2</sub> to two-dimensional Tc <sub>2</sub> B <sub>2</sub> . Physical Chemistry Chemical Physics, 2021, 23, 22086-22095.	2.8	3
50	Electronic Structures of Group III–V Element Haeckelite Compounds: A Novel Family of Semiconductors, Dirac Semimetals, and Topological Insulators. Advanced Functional Materials, 0, , 2110930.	14.9	3
51	Carbon Nanotubes Oscillation under Electric Field. Japanese Journal of Applied Physics, 2010, 49, 115103.	1.5	2
52	Symmetry Rule of the Landau Free Energy in the Phonon-Originating Phase Transition. Journal of the Physical Society of Japan, 2013, 82, 084601.	1.6	1
53	Strain Engineering to Release Trapped Hole Carriers in p-Type Haeckelite GaN. ACS Applied Electronic Materials, 2021, 3, 5257-5264.	4.3	1

<sup>2</sup>D Electrides: MXene Phase with C<sub>3</sub> Structure Unit: A Family of 2D Electrides (Adv. Funct.) Tj ETQq0 0.0 ggBT /Oyerlock 10