Fazel Shojaei

List of Publications by Year
in descending order

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Version: 2024-02-01

41 papers	2,303 citations	257450 24 h-index	289244 40 g-index
42 all docs	42 docs citations	42 times ranked	3483 citing authors

#	Article	IF	Citations
1	A first-principles and machine-learning investigation on the electronic, photocatalytic, mechanical and heat conduction properties of nanoporous C₅N monolayers. Nanoscale, 2022, 14, 4324-4333.	5.6	26
2	Comment on â€˜Biphenylene monolayer as a two-dimensional nonbenzenoid carbon allotrope: a first-principles studyâ€™. Journal of Physics Condensed Matter, 2022, 34, 248001.	1.8	0
3	A combined first-principles and machine-learning investigation on the stability, electronic, optical, and mechanical properties of novel C6N7-based nanoporous carbon nitrides. Carbon, 2022, 194, 230-239.	10.3	24
4	Comment on â€œA novel two-dimensional boron-carbon-nitride (BCN) monolayer: A first-principles insightâ€•[J. Appl. Phys. 130, 114301 (2021)]. Journal of Applied Physics, 2022, 131, 216101.	2.5	0
5	CdInGaS4: An unexplored two- dimensional materials with desirable band gap for optoelectronic devices. Journal of Alloys and Compounds, 2021, 854, 157220.	5.5	19
6	MoSi₂N₄ single-layer: a novel two-dimensional material with outstanding mechanical, thermal, electronic and optical properties. Journal Physics D: Applied Physics, 2021, 54, 155303.	2.8	160
7	Two-dimensional carbon nitride C₆N nanosheet with egg-comb-like structure and electronic properties of a semimetal. Nanotechnology, 2021, 32, 215702.	2.6	50
8	First-principles investigation of electronic, optical, mechanical and heat transport properties of pentadiamond: A comparison with diamond. Carbon Trends, 2021, 3, 100036.	3.0	16
9	Exceptional piezoelectricity, high thermal conductivity and stiffness and promising photocatalysis in two-dimensional MoSi2N4 family confirmed by first-principles. Nano Energy, 2021, 82, 105716.	16.0	303
10	High tensile strength and thermal conductivity in BeO monolayer: A first-principles study. FlatChem, 2021, 28, 100257.	5.6	24
11	Ultrahigh stiffness and anisotropic Dirac cones in BeN4 and MgN4 monolayers: a first-principles study. Materials Today Nano, 2021, 15, 100125.	4.6	23
12	Ultrahigh carrier mobility, Dirac cone and high stretchability in pyrenyl and pyrazinoquinoxaline graphdiyne/graphyne nanosheets confirmed by first-principles. Applied Surface Science, 2021, 557, 149699.	6.1	9
13	Outstandingly high thermal conductivity, elastic modulus, carrier mobility and piezoelectricity in two-dimensional semiconducting CrC2N4: a first-principles study. Materials Today Energy, 2021, 22, 100839.	4.7	19
14	As₂S₃, As₂Se₃ and As₂Te₃ nanosheets: superstretchable semiconductors with anisotropic carrier mobilities and optical properties. Journal of Materials Chemistry C, 2020, 8, 2400-2410.	5.5	45
15	Two-dimensional silicon bismotide (SiBi) monolayer with a honeycomb-like lattice: first-principles study of tuning the electronic properties. RSC Advances, 2020, 10, 31894-31900.	3.6	23
16	Nanoporous C3N4, C3N5 and C3N6 nanosheets; novel strong semiconductors with low thermal conductivities and appealing optical/electronic properties. Carbon, 2020, 167, 40-50.	10.3	72
17	High thermal conductivity in semiconducting Janus and non-Janus diamanes. Carbon, 2020, 167, 51-61.	10.3	39
18	First-principles investigation of mechanical, electronic and optical properties of H-, F- and Cl-diamane. Applied Surface Science, 2020, 528, 147035.	6.1	47

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19	Copper halide diselenium: predicted two-dimensional materials with ultrahigh anisotropic carrier mobilities. RSC Advances, 2020, 10, 8016-8026.	3.6	10
20	Silicon diphosphide (SiP2) and silicon diarsenide (SiAs2): Novel stable 2D semiconductors with high carrier mobilities, promising for water splitting photocatalysts. Materials Today Energy, 2020, 16, 100377.	4.7	33
21	Modifying the electronic and geometrical properties of mono/bi-layer graphite-like BC₂N via alkali metal (Li, Na) adsorption and intercalation: computational approach. New Journal of Chemistry, 2019, 43, 13122-13133.	2.8	9
22	Thickness-dependent bandgap and electrical properties of GeP nanosheets. Journal of Materials Chemistry A, 2019, 7, 16526-16532.	10.3	45
23	Evolutionary search for (MÂ©B₁₆)^Q (M = Scâ€“Ni; Q = 0/âˆ’1) clusters: bowl/boat vs. tubular shape. Physical Chemistry Chemical Physics, 2019, 21, 22618-22628.	2.8	18
24	Two-dimensional GeAs with a visible range band gap. Journal of Materials Chemistry A, 2018, 6, 9089-9098.	10.3	55
25	Arsenic for high-capacity lithium- and sodium-ion batteries. Nanoscale, 2018, 10, 7047-7057.	5.6	37
26	Stability Trend of Tilted Perovskites. Journal of Physical Chemistry C, 2018, 122, 15214-15219.	3.1	30
27	Electronic structure and photocatalytic band offset of few-layer GeP₂. Journal of Materials Chemistry A, 2017, 5, 22146-22155.	10.3	68
28	Partially planar BP₃with high electron mobility as a phosphorene analog. Journal of Materials Chemistry C, 2017, 5, 11267-11274.	5.5	37
29	Effect of Siâ€“Si Bonds in Silicon-Doped Î±-Phosphorene Bilayers: Two-Dimensional Layers and One-Dimensional Nanoribbons. Journal of Physical Chemistry C, 2016, 120, 17106-17114.	3.1	5
30	Photoluminescence and Photocurrents of GaS_{1â€“x}Se_x Nanobelts. Chemistry of Materials, 2016, 28, 5811-5820.	6.7	28
31	Electronic Structures and Li-Diffusion Properties of Group IVâ€“V Layered Materials: Hexagonal Germanium Phosphide and Germanium Arsenide. Journal of Physical Chemistry C, 2016, 120, 23842-23850.	3.1	41
32	Electronic structure of the germanium phosphide monolayer and Li-diffusion in its bilayer. Physical Chemistry Chemical Physics, 2016, 18, 32458-32465.	2.8	32
33	Stability and electronic structures of triazine-based carbon nitride nanotubes. RSC Advances, 2015, 5, 10892-10898.	3.6	11
34	Electronic Structure and Carrier Mobility of Two-Dimensional Î± Arsenic Phosphide. Journal of Physical Chemistry C, 2015, 119, 20210-20216.	3.1	65
35	Reversible Halide Exchange Reaction of Organometal Trihalide Perovskite Colloidal Nanocrystals for Full-Range Band Gap Tuning. Nano Letters, 2015, 15, 5191-5199.	9.1	432
36	Red-to-Ultraviolet Emission Tuning of Two-Dimensional Gallium Sulfide/Selenide. ACS Nano, 2015, 9, 9585-9593.	14.6	163

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37	Reactivity of the free and (5,5)-carbon nanotube-supported AuPt bimetallic clusters towards O₂ activation: a theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 3659-3672.	2.8	9
38	Continuous Tuning of Band Gap for Ï€-Conjugated Ni Bis(dithiolene) Complex Bilayer. Journal of Physical Chemistry C, 2014, 118, 25626-25632.	3.1	15
39	Mechanical and Electronic Properties of Ï€-Conjugated Metal Bis(dithiolene) Complex Sheets. Chemistry of Materials, 2014, 26, 2967-2974.	6.7	30
40	Tetragonal Phase Germanium Nanocrystals in Lithium Ion Batteries. ACS Nano, 2013, 7, 9075-9084.	14.6	120
41	Phase Evolution of Tin Nanocrystals in Lithium Ion Batteries. ACS Nano, 2013, 7, 11103-11111.	14.6	105