Masoud Shahrokhi

List of Publications by Year
in descending order

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53 papers	2,304 citations	186209 28 h-index	214721 47 g-index
55 all docs	55 docs citations	55 times ranked	2124 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.	2.8	26
2	Highly anisotropic mechanical and optical properties of 2D NbOX2 (XÂ=ÂCl, Br, I) revealed by first-principle. Nanotechnology, 2022, 33, 275701.	1.3	7
3	Comment on â€˜Biphenylene monolayer as a two-dimensional nonbenzenoid carbon allotrope: a first-principles studyâ€™. Journal of Physics Condensed Matter, 2022, 34, 248001.	0.7	0
4	Comment on â€œAb-initio-driven prediction of puckered penta-like PdPSeX (X=O, S, Te) Janus monolayers: Study on the electronic, optical, mechanical and photocatalytic properties [Applied Surface Science 582 (2022) 152356]â€• Applied Surface Science, 2022, , 153515.	3.1	1
5	MoSi₂N₄ single-layer: a novel two-dimensional material with outstanding mechanical, thermal, electronic and optical properties. Journal Physics D: Applied Physics, 2021, 54, 155303.	1.3	160
6	Two-dimensional carbon nitride C₆N nanosheet with egg-comb-like structure and electronic properties of a semimetal. Nanotechnology, 2021, 32, 215702.	1.3	50
7	Semiconducting Chalcogenide Alloys Based on the (Ge, Sn, Pb) (S, Se, Te) Formula with Outstanding Properties: A First-Principles Calculation Study. ACS Omega, 2021, 6, 9433-9441.	1.6	20
8	2D MoO_{3â€“x}S_x/MoS₂van der Waals Assembly: A Tunable Heterojunction with Attractive Properties for Photocatalysis. ACS Applied Materials & Interfaces, 2021, 13, 36465-36474.	4.0	29
9	Mechanical, thermal transport, electronic and photocatalytic properties of penta-PdPS, -PdPSe and -PdPTe monolayers explored by first-principles calculations. Journal of Materials Chemistry C, 2021, 10, 329-336.	2.7	14
10	Role of Intermediate Dynamics in Controlling Hydrogenation Selectivity by Heterogeneous Catalysis. ACS Omega, 2020, 5, 1270-1276.	1.6	2
11	The mechanical, electronic, optical and thermoelectric properties of two-dimensional honeycomb-like of XSb (X = Si, Ge, Sn) monolayers: a first-principles calculations. RSC Advances, 2020, 10, 30398-30405.	1.7	26
12	On the understanding of the optoelectronic properties of S-doped MoO₃ and O-doped MoS₂ bulk systems: a DFT perspective. Journal of Materials Chemistry C, 2020, 8, 9064-9074.	2.7	44
13	Optical properties of zigzag and armchair ZnO nanoribbons. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114218.	1.3	8
14	Nanoporous C3N4, C3N5 and C3N6 nanosheets; novel strong semiconductors with low thermal conductivities and appealing optical/electronic properties. Carbon, 2020, 167, 40-50.	5.4	72
15	ZnN and ZnP as novel graphene-like materials with high Li-ion storage capacities. Materials Today Energy, 2020, 16, 100392.	2.5	20
16	Prediction of C₇N₆ and C₉N₄: stable and strong porous carbon-nitride nanosheets with attractive electronic and optical properties. Journal of Materials Chemistry C, 2019, 7, 10908-10917.	2.7	57
17	Two-Dimensional SiP, SiAs, GeP and GeAs as Promising Candidates for Photocatalytic Applications. Coatings, 2019, 9, 522.	1.2	32
18	Outstanding strength, optical characteristics and thermal conductivity of graphene-like BC3 and BC6N semiconductors. Carbon, 2019, 149, 733-742.	5.4	126

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19	Nanoporous graphene: A 2D semiconductor with anisotropic mechanical, optical and thermal conduction properties. Carbon, 2019, 147, 377-384.	5.4	46
20	N-, B-, P-, Al-, As-, and Ga-graphdiyne/graphyne lattices: first-principles investigation of mechanical, optical and electronic properties. Journal of Materials Chemistry C, 2019, 7, 3025-3036.	2.7	41
21	Ti₂VGe Heuslerene: theoretical prediction of a novel 2D material. Journal of Materials Chemistry C, 2019, 7, 13559-13572.	2.7	36
22	Can fluorine and chlorine functionalization stabilize the graphene like borophene?. Computational Materials Science, 2019, 156, 56-66.	1.4	34
23	N-, P-, As-triphenylene-graphdiyne: Strong and stable 2D semiconductors with outstanding capacities as anodes for Li-ion batteries. Carbon, 2019, 141, 291-303.	5.4	73
24	Borophene hydride: a stiff 2D material with high thermal conductivity and attractive optical and electronic properties. Nanoscale, 2018, 10, 3759-3768.	2.8	109
25	Mechanical, optoelectronic and transport properties of single-layer Ca2N and Sr2N electrides. Journal of Alloys and Compounds, 2018, 739, 643-652.	2.8	14
26	Lithium halide monolayer sheets: First-principles many-body calculations. Computational Materials Science, 2018, 143, 103-111.	1.4	26
27	Structural, electronic and optical properties of Ca3Bi2: First-principles investigation. Chinese Journal of Physics, 2018, 56, 2796-2804.	2.0	2
28	Selective ensembles in supported palladium sulfide nanoparticles for alkyne semi-hydrogenation. Nature Communications, 2018, 9, 2634.	5.8	180
29	N-graphdiyne two-dimensional nanomaterials: Semiconductors with low thermal conductivity and high stretchability. Carbon, 2018, 137, 57-67.	5.4	82
30	Boronâ€“graphdiyne: a superstretchable semiconductor with low thermal conductivity and ultrahigh capacity for Li, Na and Ca ion storage. Journal of Materials Chemistry A, 2018, 6, 11022-11036.	5.2	104
31	Tuning the band gap and optical spectra of monolayer penta-graphene under in-plane biaxial strains. Optik, 2017, 136, 205-214.	1.4	34
32	Anisotropic mechanical and optical response and negative Poissonâ€™s ratio in Mo₂C nanomembranes revealed by first-principles simulations. Nanotechnology, 2017, 28, 115705.	1.3	57
33	New two-dimensional boron nitride allotropes with attractive electronic and optical properties. Solid State Communications, 2017, 253, 51-56.	0.9	53
34	Quasi-particle energies and optical excitations of novel porous graphene phases from first-principles many-body calculations. Diamond and Related Materials, 2017, 77, 35-40.	1.8	25
35	Hybrid Palladium Nanoparticles for Direct Hydrogen Peroxide Synthesis: The Key Role of the Ligand. Angewandte Chemie, 2017, 129, 1801-1805.	1.6	36
36	Hybrid Palladium Nanoparticles for Direct Hydrogen Peroxide Synthesis: The Key Role of the Ligand. Angewandte Chemie - International Edition, 2017, 56, 1775-1779.	7.2	78

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37	Theoretical realization of Mo2P; a novel stable 2D material with superionic conductivity and attractive optical properties. Applied Materials Today, 2017, 9, 292-299.	2.3	43
38	Electronic, optical and thermal properties of highly stretchable 2D carbon Ene-yne graphyne. Carbon, 2017, 123, 344-353.	5.4	46
39	Tuning the band gap and optical spectra of silicon-doped graphene: Many-body effects and excitonic states. Journal of Alloys and Compounds, 2017, 693, 1185-1196.	2.8	119
40	Quasi-particle energies and optical excitations of wurtzite BeO and its nanosheet. Journal of Alloys and Compounds, 2016, 682, 254-262.	2.8	63
41	Quasi-particle energies and optical excitations of ZnS monolayer honeycomb structure. Applied Surface Science, 2016, 390, 377-384.	3.1	57
42	Structural, electronic and magnetic properties of (N, C)-codoped ZnO nanotube: First principles study. International Journal of Modern Physics C, 2015, 26, 1550130.	0.8	15
43	Structural, electronic and magnetic properties of Fe, Co, Ni monatomic nanochains encapsulated in BeO nanotubes bundle. EPJ Applied Physics, 2014, 65, 20402.	0.3	11
44	Theoretical exploration of structural, electro-optical and magnetic properties of gallium-doped silicon carbide nanotubes. Superlattices and Microstructures, 2014, 73, 185-192.	1.4	20
45	Density functional investigation of structural, electronic and magnetic properties of Cu-codoped ZnO nanotubes. EPJ Applied Physics, 2014, 67, 20403.	0.3	10
46	Structural, electronic and optical properties of nanotubes: First principles study. Journal of Physics and Chemistry of Solids, 2013, 74, 1063-1068.	1.9	23
47	Magnetic semiconductor and metalâ€“semiconductor junction by nanoparticles encapsulated in beryllium oxygen nanotube. Journal of Magnetism and Magnetic Materials, 2013, 344, 162-166.	1.0	8
48	Optical properties of BeO nanotubes: Ab initio study. Solid State Communications, 2013, 156, 1-7.	0.9	30
49	First principle study of the structural, electronic and magnetic properties of Fe, Co, Ni atomic nanochains encapsulated in single walled and double walled beryllium oxygen nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 47, 40-45.	1.3	19
50	Structural, electronic and magnetic properties of Fe and Co monatomic nanochains encapsulated in BN nanotube bundle. EPJ Applied Physics, 2013, 62, 30402.	0.3	14
51	First principles study of the structural, electronic and optical properties of nanotube. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1760-1765.	1.3	24
52	Structural, magnetic, electronic and optical properties of iron cluster (Fe6) decorated boron nitride sheet. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 46, 182-188.	1.3	26
53	Ab initio calculations of optical properties of B2C graphene sheet. Solid State Communications, 2012, 152, 1012-1017.	0.9	46