

Bohayra Mortazavi

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134
papers

5,190
citations

42
h-index

67
g-index

144
ext. papers

6,360
ext. citations

5.9
avg, IF

6.77
L-index

#	Paper	IF	Citations
134	Thermal conductivity and tensile response of defective graphene: A molecular dynamics study. <i>Carbon</i> , 2013 , 63, 460-470	10.4	186
133	Ultra high stiffness and thermal conductivity of graphene like C3N. <i>Carbon</i> , 2017 , 118, 25-34	10.4	182
132	Application of silicene, germanene and stanene for Na or Li ion storage: A theoretical investigation. <i>Electrochimica Acta</i> , 2016 , 213, 865-870	6.7	171
131	Borophene as an anode material for Ca, Mg, Na or Li ion storage: A first-principle study. <i>Journal of Power Sources</i> , 2016 , 329, 456-461	8.9	147
130	Interphase effect on the elastic and thermal conductivity response of polymer nanocomposite materials: 3D finite element study. <i>Computational Materials Science</i> , 2013 , 69, 100-106	3.2	124
129	First-principles investigation of mechanical properties of silicene, germanene and stanene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2017 , 87, 228-232	3	118
128	Combined molecular dynamics-finite element multiscale modeling of thermal conduction in graphene epoxy nanocomposites. <i>Carbon</i> , 2013 , 60, 356-365	10.4	115
127	Modeling of two-phase random composite materials by finite element, Mori-Tanaka and strong contrast methods. <i>Composites Part B: Engineering</i> , 2013 , 45, 1117-1125	10	114
126	Mechanical responses of borophene sheets: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 27405-27413	3.6	111
125	Graphene or h-BN paraffin composite structures for the thermal management of Li-ion batteries: A multiscale investigation. <i>Applied Energy</i> , 2017 , 202, 323-334	10.7	105
124	Thermal conductivity and mechanical properties of nitrogenated holey graphene. <i>Carbon</i> , 2016 , 106, 1-8	10.4	101
123	Investigation of tensile response and thermal conductivity of boron-nitride nanosheets using molecular dynamics simulations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2012 , 44, 1846-1852	10.4	100
122	Adsorption of Metallic, Metalloidal, and Nonmetallic Adatoms on Two-Dimensional C3N. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 18575-18583	3.8	97
121	Outstanding strength, optical characteristics and thermal conductivity of graphene-like BC3 and BC6N semiconductors. <i>Carbon</i> , 2019 , 149, 733-742	10.4	93
120	Nitrogen doping and curvature effects on thermal conductivity of graphene: A non-equilibrium molecular dynamics study. <i>Solid State Communications</i> , 2012 , 152, 261-264	1.6	90
119	Modelling heat conduction in polycrystalline hexagonal boron-nitride films. <i>Scientific Reports</i> , 2015 , 5, 13228	4.9	90
118	Multiscale modeling of thermal conductivity of polycrystalline graphene sheets. <i>Nanoscale</i> , 2014 , 6, 3344-3352	5.2	88

117	Multiscale modeling of heat conduction in graphene laminates. <i>Carbon</i> , 2015 , 85, 1-7	10.4	88
116	Mechanical properties and thermal conductivity of graphitic carbon nitride: A molecular dynamics study. <i>Computational Materials Science</i> , 2015 , 99, 285-289	3.2	87
115	Flat borophene films as anode materials for Mg, Na or Li-ion batteries with ultra high capacities: A first-principles study. <i>Applied Materials Today</i> , 2017 , 8, 60-67	6.6	86
114	Atomistic modeling of mechanical properties of polycrystalline graphene. <i>Nanotechnology</i> , 2014 , 25, 215704	3.4	86
113	Borophene hydride: a stiff 2D material with high thermal conductivity and attractive optical and electronic properties. <i>Nanoscale</i> , 2018 , 10, 3759-3768	7.7	83
112	Mechanical properties of polycrystalline boron-nitride nanosheets. <i>RSC Advances</i> , 2014 , 4, 19137-19143	3.7	83
111	Boron-graphdiyne: a superstretchable semiconductor with low thermal conductivity and ultrahigh capacity for Li, Na and Ca ion storage. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 11022-11036	13	80
110	Molecular dynamics study on the thermal conductivity and mechanical properties of boron doped graphene. <i>Solid State Communications</i> , 2012 , 152, 1503-1507	1.6	75
109	Nitrogen doping and vacancy effects on the mechanical properties of graphene: A molecular dynamics study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 1146-1153	2.3	71
108	Amorphized graphene: A stiff material with low thermal conductivity. <i>Carbon</i> , 2016 , 103, 318-326	10.4	70
107	Exceptional piezoelectricity, high thermal conductivity and stiffness and promising photocatalysis in two-dimensional MoSi ₂ N ₄ family confirmed by first-principles. <i>Nano Energy</i> , 2021 , 82, 105716	17.1	70
106	N-graphdiyne two-dimensional nanomaterials: Semiconductors with low thermal conductivity and high stretchability. <i>Carbon</i> , 2018 , 137, 57-67	10.4	67
105	Experimental and multiscale modeling of thermal conductivity and elastic properties of PLA/expanded graphite polymer nanocomposites. <i>Thermochimica Acta</i> , 2013 , 552, 106-113	2.9	63
104	N-, P-, As-triphenylene-graphdiyne: Strong and stable 2D semiconductors with outstanding capacities as anodes for Li-ion batteries. <i>Carbon</i> , 2019 , 141, 291-303	10.4	63
103	Machine-learning interatomic potentials enable first-principles multiscale modeling of lattice thermal conductivity in graphene/borophene heterostructures. <i>Materials Horizons</i> , 2020 , 7, 2359-2367	14.4	62
102	Enhancement in hydrogen storage capacities of light metal functionalized Boron-graphdiyne nanosheets. <i>Carbon</i> , 2019 , 147, 199-205	10.4	59
101	2D Hydrogenated graphene-like borophene as a high capacity anode material for improved Li/Na ion batteries: A first principles study. <i>Materials Today Energy</i> , 2018 , 8, 22-28	7	58
100	Thickness and chirality effects on tensile behavior of few-layer graphene by molecular dynamics simulations. <i>Computational Materials Science</i> , 2012 , 53, 298-302	3.2	58

99	Mechanical response of all-MoS ₂ single-layer heterostructures: a ReaxFF investigation. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 23695-701	3.6	55
98	Anisotropic thermal conductivity and mechanical properties of phagraphene: a molecular dynamics study. <i>RSC Advances</i> , 2016 , 6, 57773-57779	3.7	53
97	Electrical and Thermal Transport in Coplanar Polycrystalline Graphene-hBN Heterostructures. <i>Nano Letters</i> , 2017 , 17, 1660-1664	11.5	52
96	Alignments and network of graphite fillers to improve thermal conductivity of epoxy-based composites. <i>International Journal of Heat and Mass Transfer</i> , 2015 , 89, 505-513	4.9	52
95	Tunable electronic and magnetic properties of graphene/carbon-nitride van der Waals heterostructures. <i>Applied Surface Science</i> , 2020 , 505, 144450	6.7	47
94	Exploring phononic properties of two-dimensional materials using machine learning interatomic potentials. <i>Applied Materials Today</i> , 2020 , 20, 100685	6.6	46
93	Accelerating first-principles estimation of thermal conductivity by machine-learning interatomic potentials: A MTP/ShengBTE solution. <i>Computer Physics Communications</i> , 2021 , 258, 107583	4.2	44
92	Anisotropic mechanical and optical response and negative Poisson's ratio in MoC nanomembranes revealed by first-principles simulations. <i>Nanotechnology</i> , 2017 , 28, 115705	3.4	41
91	Modeling Kapitza resistance of two-phase composite material. <i>Composite Structures</i> , 2016 , 152, 939-946	5.3	41
90	Anomalous strain effect on the thermal conductivity of borophene: a reactive molecular dynamics study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2017 , 93, 202-207	3	40
89	Mechanical properties of borophene films: a reactive molecular dynamics investigation. <i>Nanotechnology</i> , 2016 , 27, 445709	3.4	40
88	Theoretical Investigation: 2D N-Graphdiyne Nanosheets as Promising Anode Materials for Li/Na Rechargeable Storage Devices. <i>ACS Applied Nano Materials</i> , 2019 , 2, 127-135	5.6	40
87	Prediction of C ₇ N ₆ and C ₉ N ₄ : stable and strong porous carbon-nitride nanosheets with attractive electronic and optical properties. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 10908-10917	7.1	37
86	Three-dimensional reconstruction and homogenization of heterogeneous materials using statistical correlation functions and FEM. <i>Computational Materials Science</i> , 2012 , 51, 372-379	3.2	37
85	N-, B-, P-, Al-, As-, and Ga-graphdiyne/graphyne lattices: first-principles investigation of mechanical, optical and electronic properties. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 3025-3036	7.1	35
84	Electronic, optical and thermal properties of highly stretchable 2D carbon Ene-yne graphyne. <i>Carbon</i> , 2017 , 123, 344-353	10.4	35
83	Nanoporous C ₃ N ₄ , C ₃ N ₅ and C ₃ N ₆ nanosheets; novel strong semiconductors with low thermal conductivities and appealing optical/electronic properties. <i>Carbon</i> , 2020 , 167, 40-50	10.4	34
82	Nanoporous graphene: A 2D semiconductor with anisotropic mechanical, optical and thermal conduction properties. <i>Carbon</i> , 2019 , 147, 377-384	10.4	33

81	First-Principles Multiscale Modeling of Mechanical Properties in Graphene/Borophene Heterostructures Empowered by Machine-Learning Interatomic Potentials. <i>Advanced Materials</i> , 2021 , 33, e2102807	24	33
80	Edge-Grafted Molecular Junctions between Graphene Nanoplatelets: Applied Chemistry to Enhance Heat Transfer in Nanomaterials. <i>Advanced Functional Materials</i> , 2018 , 28, 1706954	15.6	32
79	Theoretical realization of Mo2P; a novel stable 2D material with superionic conductivity and attractive optical properties. <i>Applied Materials Today</i> , 2017 , 9, 292-299	6.6	32
78	Thermal conductivity of MoS ₂ polycrystalline nanomembranes. <i>2D Materials</i> , 2016 , 3, 035016	5.9	32
77	Anisotropic mechanical properties and strain tuneable band-gap in single-layer SiP, SiAs, GeP and GeAs. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018 , 103, 273-278	3	31
76	New two-dimensional boron nitride allotropes with attractive electronic and optical properties. <i>Solid State Communications</i> , 2017 , 253, 51-56	1.6	29
75	Strong thermal transport along polycrystalline transition metal dichalcogenides revealed by multiscale modeling for MoS ₂ . <i>Applied Materials Today</i> , 2017 , 7, 67-76	6.6	29
74	Carbon ene-yne graphyne monolayer as an outstanding anode material for Li/Na ion batteries. <i>Applied Materials Today</i> , 2018 , 10, 115-121	6.6	29
73	A structural insight into mechanical strength of graphene-like carbon and carbon nitride networks. <i>Nanotechnology</i> , 2017 , 28, 055707	3.4	28
72	Boron Monochalcogenides; Stable and Strong Two-Dimensional Wide Band-Gap Semiconductors. <i>Energies</i> , 2018 , 11, 1573	3.1	28
71	Theoretical realization of two-dimensional M ₃ (C ₆ X ₆) ₂ (M = Co, Cr, Cu, Fe, Mn, Ni, Pd, Rh and X = O, S, Se) metal-organic frameworks. <i>Applied Materials Today</i> , 2019 , 15, 405-415	6.6	27
70	Embedding of atoms into the nanopore sites of the CN and CN porous carbon nitride monolayers with tunable electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 6418-6433	3.6	27
69	As ₂ S ₃ , As ₂ Se ₃ and As ₂ Te ₃ nanosheets: superstretchable semiconductors with anisotropic carrier mobilities and optical properties. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 2400-2410	7.1	27
68	Record Low Thermal Conductivity of Polycrystalline MoS ₂ Films: Tuning the Thermal Conductivity by Grain Orientation. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 37905-37911	9.5	26
67	Band gap and magnetism engineering in Dirac half-metallic Na ₂ C nanosheet via layer thickness, strain and point defects. <i>Journal of Magnetism and Magnetic Materials</i> , 2019 , 491, 165565	2.8	26
66	A first-principles study on the effect of oxygen content on the structural and electronic properties of silicon suboxide as anode material for lithium ion batteries. <i>Journal of Power Sources</i> , 2016 , 307, 657-664	8.9	25
65	Metamorphosis in carbon network: From penta-graphene to biphenylene under uniaxial tension. <i>FlatChem</i> , 2017 , 1, 65-73	5.1	24
64	Application of two-dimensional materials as anodes for rechargeable metal-ion batteries: A comprehensive perspective from density functional theory simulations. <i>Energy Storage Materials</i> , 2021 , 35, 203-282	19.4	23

63	First-principles investigation of mechanical, electronic and optical properties of H-, F- and Cl-diamane. <i>Applied Surface Science</i> , 2020 , 528, 147035	6.7	22
62	High thermal conductivity in semiconducting Janus and non-Janus diamanes. <i>Carbon</i> , 2020 , 167, 51-61	10.4	21
61	Mechanical responses of two-dimensional MoTe ₂ ; pristine 2H, 1T and 1T' and 1T'/2H heterostructure. <i>Extreme Mechanics Letters</i> , 2018 , 20, 65-72	3.9	21
60	Molecular Dynamics Investigation of Loading Rate Effects on Mechanical-Failure Behaviour of FCC Metals. <i>Journal of Computational and Theoretical Nanoscience</i> , 2009 , 6, 644-652	0.3	21
59	Ab initio prediction of semiconductivity in a novel two-dimensional SbX (X= S, Se, Te) monolayers with orthorhombic structure. <i>Scientific Reports</i> , 2021 , 11, 10366	4.9	20
58	Lithium halide monolayer sheets: First-principles many-body calculations. <i>Computational Materials Science</i> , 2018 , 143, 103-111	3.2	20
57	Silicon diphosphide (SiP ₂) and silicon diarsenide (SiAs ₂): Novel stable 2D semiconductors with high carrier mobilities, promising for water splitting photocatalysts. <i>Materials Today Energy</i> , 2020 , 16, 100377	7	19
56	Thermal and electronic transport characteristics of highly stretchable graphene kirigami. <i>Nanoscale</i> , 2017 , 9, 16329-16341	7.7	19
55	A computational and experimental investigation of the mechanical properties of single ZnTe nanowires. <i>Nanoscale</i> , 2012 , 4, 897-903	7.7	19
54	A Study on the Nanoindentation Behaviour of Single Crystal Silicon Using Hybrid MD-FE Method. <i>Advanced Materials Research</i> , 2008 , 32, 259-262	0.5	19
53	Thermal bridging of graphene nanosheets via covalent molecular junctions: A non-equilibrium Green's functions density functional tight-binding study. <i>Nano Research</i> , 2019 , 12, 791-799	10	19
52	Multiscale modelling of heat conduction in all-MoS ₂ single-layer heterostructures. <i>RSC Advances</i> , 2017 , 7, 11135-11141	3.7	17
51	Two-Dimensional SiP, SiAs, GeP and GeAs as Promising Candidates for Photocatalytic Applications. <i>Coatings</i> , 2019 , 9, 522	2.9	16
50	Efficient machine-learning based interatomic potentials for exploring thermal conductivity in two-dimensional materials. <i>JPhys Materials</i> , 2020 , 3, 02LT02	4.2	16
49	ZnN and ZnP as novel graphene-like materials with high Li-ion storage capacities. <i>Materials Today Energy</i> , 2020 , 16, 100392	7	16
48	Tuning Thermal Transport in C ₃ N Monolayers by Adding and Removing Carbon Atoms. <i>Physical Review Applied</i> , 2018 , 10,	4.3	16
47	Ultrahigh thermal conductivity and strength in direct-gap semiconducting graphene-like BC ₆ N: A first-principles and classical investigation. <i>Carbon</i> , 2021 , 182, 373-383	10.4	16
46	Thermal conductivity of ZnTe nanowires. <i>Journal of Applied Physics</i> , 2013 , 114, 134314	2.5	15

45	A statistical approach for the evaluation of mechanical properties of silica/epoxy nanocomposite: Verification by experiments. <i>Computational Materials Science</i> , 2012 , 59, 108-113	3.2	15
44	Point Defects in a Two-Dimensional ZnSnN ₂ Nanosheet: A First-Principles Study on the Electronic and Magnetic Properties. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 13067-13075	3.8	15
43	First-principles investigation of Ag-, Co-, Cr-, Cu-, Fe-, Mn-, Ni-, Pd- and Rh-hexaaminobenzene 2D metal-organic frameworks. <i>Materials Today Energy</i> , 2018 , 10, 336-342	7	15
42	Tunable electronic properties of the dynamically stable layered mineral PtHgSe (Jacutingaite). <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 24471-24479	3.6	14
41	Machine learning assisted multiscale modeling of composite phase change materials for Li-ion batteries thermal management. <i>International Journal of Heat and Mass Transfer</i> , 2021 , 172, 121199	4.9	14
40	Hydrogenation and defect formation control the strength and ductility of MoS ₂ nanosheets: Reactive molecular dynamics simulation. <i>Extreme Mechanics Letters</i> , 2018 , 22, 157-164	3.9	13
39	Intelligent on-demand design of phononic metamaterials. <i>Nanophotonics</i> , 2022 , 11, 439-460	6.3	11
38	First-principles investigation of electronic, optical, mechanical and heat transport properties of pentadiamond: A comparison with diamond. <i>Carbon Trends</i> , 2021 , 3, 100036	0	9
37	Atomistic-Continuum Modeling of the Mechanical Properties of Silica/Epoxy Nanocomposite. <i>Journal of Engineering Materials and Technology, Transactions of the ASME</i> , 2012 , 134,	1.8	8
36	Electro-optical and mechanical properties of Zinc antimonide (ZnSb) monolayer and bilayer: A first-principles study. <i>Applied Surface Science</i> , 2021 , 540, 148289	6.7	8
35	First-principles investigation of electronic, mechanical and thermoelectric properties of graphene-like XBi (X = Si, Ge, Sn) monolayers. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 12471-12478	3.6	8
34	Exploration of mechanical, thermal conductivity and electromechanical properties of graphene nanoribbon springs. <i>Nanoscale Advances</i> , 2020 , 2, 3394-3403	5.1	7
33	Mechanical, optoelectronic and transport properties of single-layer Ca ₂ N and Sr ₂ N electrides. <i>Journal of Alloys and Compounds</i> , 2018 , 739, 643-652	5.7	7
32	Two-dimensional PdPS and PdPSe nanosheets: Novel promising sensing platforms for harmful gas molecules. <i>Applied Surface Science</i> , 2022 , 579, 152115	6.7	7
31	New group V graphyne: two-dimensional direct semiconductors with remarkable carrier mobilities, thermoelectric performance, and thermal stability. <i>Materials Today Physics</i> , 2020 , 12, 100164	8	7
30	Electronic, optical and thermoelectric properties of boron-doped nitrogenated holey graphene. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 21147-21157	3.6	7
29	Effect of straining graphene on nanopore creation using Si cluster bombardment: A reactive atomistic investigation. <i>Journal of Applied Physics</i> , 2016 , 120, 225108	2.5	7
28	Ultrahigh stiffness and anisotropic Dirac cones in BeN ₄ and MgN ₄ monolayers: a first-principles study. <i>Materials Today Nano</i> , 2021 , 15, 100125	9.7	7

27	Aromatic molecular junctions between graphene sheets: a molecular dynamics screening for enhanced thermal conductance.. <i>RSC Advances</i> , 2019 , 9, 15573-15581	3.7	6
26	Exploring thermal expansion of carbon-based nanosheets by machine-learning interatomic potentials. <i>Carbon</i> , 2022 , 186, 501-508	10.4	6
25	High tensile strength and thermal conductivity in BeO monolayer: A first-principles study. <i>FlatChem</i> , 2021 , 28, 100257	5.1	6
24	Outstandingly high thermal conductivity, elastic modulus, carrier mobility and piezoelectricity in two-dimensional semiconducting CrC ₂ N ₄ : a first-principles study. <i>Materials Today Energy</i> , 2021 , 22, 100839	7.7	6
23	Mechanical, thermal transport, electronic and photocatalytic properties of penta-PdPS, -PdPSe and -PdPTe monolayers explored by first-principles calculations. <i>Journal of Materials Chemistry C</i> , 2021 , 10, 329-336	7.1	5
22	Ultrahigh carrier mobility, Dirac cone and high stretchability in pyrenyl and pyrazinoquinoxaline graphdiyne/graphyne nanosheets confirmed by first-principles. <i>Applied Surface Science</i> , 2021 , 557, 149699	6.7	4
21	Effective Parameters on the Stress-Strain Curve of Nylon 66/Clay Nanocomposite Using FEM. <i>Strain</i> , 2011 , 47, e442-e446	1.7	3
20	Monolayer C ₇ N ₆ : Room-temperature excitons with large binding energies and high thermal conductivities. <i>Physical Review Materials</i> , 2020 , 4,	3.2	3
19	A machine-learning-based investigation on the mechanical/failure response and thermal conductivity of semiconducting BC ₂ N monolayers. <i>Carbon</i> , 2022 , 188, 431-441	10.4	3
18	A Multiscale Investigation on the Thermal Transport in Polydimethylsiloxane Nanocomposites: Graphene vs. Borophene. <i>Nanomaterials</i> , 2021 , 11,	5.4	3
17	Exploring tensile piezoelectricity and bending flexoelectricity of diamane monolayers by machine learning. <i>Carbon</i> , 2021 , 185, 558-567	10.4	3
16	Outstanding thermal conductivity and mechanical properties in the direct gap semiconducting penta-NiN ₂ monolayer confirmed by first-principles. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022 , 140, 115221	3	3
15	Annealing effect on the thermal conductivity of thermoelectric ZnTe nanowires. <i>Materials Letters</i> , 2014 , 135, 87-91	3.3	2
14	Nanopore creation in MoS ₂ and graphene monolayers by nanoparticles impact: a reactive molecular dynamics study. <i>Applied Physics A: Materials Science and Processing</i> , 2021 , 127, 1	2.6	2
13	Molecular Dynamics Modeling of Mechanical Properties of Polymer Nanocomposites Reinforced by C ₇ N ₆ Nanosheet. <i>Surfaces</i> , 2021 , 4, 240-254	2.9	2
12	Molecular Junctions Enhancing Thermal Transport within Graphene Polymer Nanocomposite: A Molecular Dynamics Study. <i>Nanomaterials</i> , 2021 , 11,	5.4	2
11	A first-principles and machine-learning investigation on the electronic, photocatalytic, mechanical and heat conduction properties of nanoporous CN monolayers.. <i>Nanoscale</i> , 2022 ,	7.7	2
10	Anisotropic charge transport in 1D and 2D BeN ₄ and MgN ₄ nanomaterials: A first-principles study. <i>FlatChem</i> , 2022 , 31, 100327	5.1	1

9	Exploring the mechanical properties of two-dimensional carbon-nitride polymer nanocomposites by molecular dynamics simulations. <i>Composite Structures</i> , 2021 , 115004	5.3	o
8	Comment on MoSi_2N_4 single-layer: a novel two-dimensional material with outstanding mechanical, thermal, electronic and optical properties [Journal Physics D: Applied Physics, 2022 , 55, 068001	3	o
7	Anisotropic mechanical response, high negative thermal expansion, and outstanding dynamical stability of biphenylene monolayer revealed by machine-learning interatomic potentials. <i>FlatChem</i> , 2022 , 32, 100347	5.1	o
6	A combined first-principles and machine-learning investigation on the stability, electronic, optical, and mechanical properties of novel C_6N_7 -based nanoporous carbon nitrides. <i>Carbon</i> , 2022 , 194, 230-239 ^{10.4}		o
5	Comment on Ab-initio -driven prediction of puckered penta-like PdPSeX ($\text{X}=\text{O}, \text{S}, \text{Te}$) Janus monolayers: Study on the electronic, optical, mechanical and photocatalytic properties [Applied Surface Science 582 (2022) 152356] [Applied Surface Science, 2022 , 153515	6.7	o
4	Investigation of Mechanical Properties of Silica/Epoxy Nano-Composites by Molecular Dynamics and Finite Element Modeling 2011 , 117-120		
3	Loading Rate Effects on Mechanical Response of Ag, Ni, Al and Cu at Nano-Scale. <i>Strain</i> , 2011 , 47, 183-187		
2	Monoelemental two-dimensional iodine nanosheets: a first-principles study of the electronic and optical properties. <i>Journal Physics D: Applied Physics</i> , 2022 , 55, 135104	3	
1	Comment on A novel two-dimensional boron-carbon-nitride (BCN) monolayer: A first-principles insight [J. Appl. Phys. 130, 114301 (2021)]. <i>Journal of Applied Physics</i> , 2022 , 131, 216101	2.5	