Bohayra Mortazavi

List of Publications by Year in Descending Order

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	Anisotropic charge transport in 1D and 2D BeN4 and MgN4 nanomaterials: A first-principles study. *FlatChem*, **2022**, 31, 100327	5.1	1
133	Intelligent on-demand design of phononic metamaterials. *Nanophotonics*, **2022**, 11, 439-460	6.3	11
132	Two-dimensional PdPS and PdPSe nanosheets: Novel promising sensing platforms for harmful gas molecules. *Applied Surface Science*, **2022**, 579, 152115	6.7	7
131	A machine-learning-based investigation on the mechanical/failure response and thermal conductivity of semiconducting BC2N monolayers. *Carbon*, **2022**, 188, 431-441	10.4	3
130	Comment on "MoSi2N4 single-layer: a novel two-dimensional material with outstanding mechanical, thermal, electronic and optical properties". *Journal Physics D: Applied Physics*, **2022**, 55, 068001	3	0
129	Exploring thermal expansion of carbon-based nanosheets by machine-learning interatomic potentials. *Carbon*, **2022**, 186, 501-508	10.4	6
128	A first-principles and machine-learning investigation on the electronic, photocatalytic, mechanical and heat conduction properties of nanoporous CN monolayers.. *Nanoscale*, **2022**,	7.7	2
127	Anisotropic mechanical response, high negative thermal expansion, and outstanding dynamical stability of biphenylene monolayer revealed by machine-learning interatomic potentials. *FlatChem*, **2022**, 32, 100347	5.1	0
126	Outstanding thermal conductivity and mechanical properties in the direct gap semiconducting penta-NiN2 monolayer confirmed by first-principles. *Physica E: Low-Dimensional Systems and Nanostructures*, **2022**, 140, 115221	3	3
125	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	10.4	0
124	Monoelemental two-dimensional iodinene nanosheets: a first-principles study of the electronic and optical properties. *Journal Physics D: Applied Physics*, **2022**, 55, 135104	3	
123	Comment on "Ab-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]". *Applied Surface Science*, **2022**, 153515	6.7	0
122	Comment on "A novel two-dimensional boron-carbon-nitride (BCN) monolayer: A first-principles insight [J. Appl. Phys. 130, 114301 (2021)]. *Journal of Applied Physics*, **2022**, 131, 216101	2.5	
121	Exploring the mechanical properties of two-dimensional carbon-nitride polymer nanocomposites by molecular dynamics simulations. *Composite Structures*, **2021**, 115004	5.3	0
120	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	7.1	5
119	First-principles investigation of electronic, optical, mechanical and heat transport properties of pentadiamond: A comparison with diamond. *Carbon Trends*, **2021**, 3, 100036	0	9
118	Exceptional piezoelectricity, high thermal conductivity and stiffness and promising photocatalysis in two-dimensional MoSi2N4 family confirmed by first-principles. *Nano Energy*, **2021**, 82, 105716	17.1	70

117	Ab initio prediction of semiconductivity in a novel two-dimensional SbX (X= S, Se, Te) monolayers with orthorhombic structure. *Scientific Reports*, **2021**, 11, 10366	4.9	20
116	A Multiscale Investigation on the Thermal Transport in Polydimethylsiloxane Nanocomposites: Graphene vs. Borophene. *Nanomaterials*, **2021**, 11,	5.4	3
115	Machine learning assisted multiscale modeling of composite phase change materials for Li-ion batteries□thermal management. *International Journal of Heat and Mass Transfer*, **2021**, 172, 121199	4.9	14
114	Nanopore creation in MoS2 and graphene monolayers by nanoparticles impact: a reactive molecular dynamics study. *Applied Physics A: Materials Science and Processing*, **2021**, 127, 1	2.6	2
113	Point Defects in a Two-Dimensional ZnSnN2 Nanosheet: A First-Principles Study on the Electronic and Magnetic Properties. *Journal of Physical Chemistry C*, **2021**, 125, 13067-13075	3.8	15
112	Accelerating first-principles estimation of thermal conductivity by machine-learning interatomic potentials: A MTP/ShengBTE solution. *Computer Physics Communications*, **2021**, 258, 107583	4.2	44
111	Application of two-dimensional materials as anodes for rechargeable metal-ion batteries: A comprehensive perspective from density functional theory simulations. *Energy Storage Materials*, **2021**, 35, 203-282	19.4	23
110	Electro-optical and mechanical properties of Zinc antimonide (ZnSb) monolayer and bilayer: A first-principles study. *Applied Surface Science*, **2021**, 540, 148289	6.7	8
109	High tensile strength and thermal conductivity in BeO monolayer: A first-principles study. *FlatChem* , **2021**, 28, 100257	5.1	6
108	First-Principles Multiscale Modeling of Mechanical Properties in Graphene/Borophene Heterostructures Empowered by Machine-Learning Interatomic Potentials. *Advanced Materials*, **2021**, 33, e2102807	24	33
107	Ultrahigh stiffness and anisotropic Dirac cones in BeN4 and MgN4 monolayers: a first-principles study. *Materials Today Nano*, **2021**, 15, 100125	9.7	7
106	Molecular Dynamics Modeling of Mechanical Properties of Polymer Nanocomposites Reinforced by C7N6 Nanosheet. *Surfaces*, **2021**, 4, 240-254	2.9	2
105	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	6.7	4
104	Ultrahigh thermal conductivity and strength in direct-gap semiconducting graphene-like BC6N: A first-principles and classical investigation. *Carbon*, **2021**, 182, 373-383	10.4	16
103	Molecular Junctions Enhancing Thermal Transport within Graphene Polymer Nanocomposite: A Molecular Dynamics Study. *Nanomaterials*, **2021**, 11,	5.4	2
102	Exploring tensile piezoelectricity and bending flexoelectricity of diamane monolayers by machine learning. *Carbon*, **2021**, 185, 558-567	10.4	3
101	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	7	6
100	First-principles investigation of electronic, mechanical and thermoelectric properties of graphene-like XBi (X = Si, Ge, Sn) monolayers. *Physical Chemistry Chemical Physics*, **2021**, 23, 12471-12478	3.6	8

99	Exploring phononic properties of two-dimensional materials using machine learning interatomic potentials. *Applied Materials Today*, **2020**, 20, 100685	6.6	46
98	Nanoporous C3N4, C3N5 and C3N6 nanosheets; novel strong semiconductors with low thermal conductivities and appealing optical/electronic properties. *Carbon*, **2020**, 167, 40-50	10.4	34
97	High thermal conductivity in semiconducting Janus and non-Janus diamanes. *Carbon*, **2020**, 167, 51-61	10.4	21
96	Machine-learning interatomic potentials enable first-principles multiscale modeling of lattice thermal conductivity in graphene/borophene heterostructures. *Materials Horizons*, **2020**, 7, 2359-2367	14.4	62
95	Efficient machine-learning based interatomic potentialsfor exploring thermal conductivity in two-dimensional materials. *JPhys Materials*, **2020**, 3, 02LT02	4.2	16
94	First-principles investigation of mechanical, electronic and optical properties of H-, F- and Cl-diamane. *Applied Surface Science*, **2020**, 528, 147035	6.7	22
93	Exploration of mechanical, thermal conductivity and electromechanical properties of graphene nanoribbon springs. *Nanoscale Advances*, **2020**, 2, 3394-3403	5.1	7
92	ZnN and ZnP as novel graphene-like materials with high Li-ion storage capacities. *Materials Today Energy*, **2020**, 16, 100392	7	16
91	Embedding of atoms into the nanopore sites of the CN and CN porous carbon nitride monolayers with tunable electronic properties. *Physical Chemistry Chemical Physics*, **2020**, 22, 6418-6433	3.6	27
90	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	7	19
89	Monolayer C7N6: Room-temperature excitons with large binding energies and high thermal conductivities. *Physical Review Materials*, **2020**, 4,	3.2	3
88	As2S3, As2Se3 and As2Te3 nanosheets: superstretchable semiconductors with anisotropic carrier mobilities and optical properties. *Journal of Materials Chemistry C*, **2020**, 8, 2400-2410	7.1	27
87	Tunable electronic and magnetic properties of graphene/carbon-nitride van der Waals heterostructures. *Applied Surface Science*, **2020**, 505, 144450	6.7	47
86	New group V graphyne: two-dimensional direct semiconductors with remarkable carrier mobilities, thermoelectric performance, and thermal stability. *Materials Today Physics*, **2020**, 12, 100164	8	7
85	Tunable electronic properties of the dynamically stable layered mineral PtHgSe (Jacutingaite). *Physical Chemistry Chemical Physics*, **2020**, 22, 24471-24479	3.6	14
84	Electronic, optical and thermoelectric properties of boron-doped nitrogenated holey graphene. *Physical Chemistry Chemical Physics*, **2020**, 22, 21147-21157	3.6	7
83	Two-Dimensional SiP, SiAs, GeP and GeAs as Promising Candidates for Photocatalytic Applications. *Coatings*, **2019**, 9, 522	2.9	16
82	Outstanding strength, optical characteristics and thermal conductivity of graphene-like BC3 and BC6N semiconductors. *Carbon*, **2019**, 149, 733-742	10.4	93

81	Nanoporous graphene: A 2D semiconductor with anisotropic mechanical, optical and thermal conduction properties. *Carbon*, **2019**, 147, 377-384	10.4	33
80	Enhancement in hydrogen storage capacities of light metal functionalized Boron□Graphdiyne nanosheets. *Carbon*, **2019**, 147, 199-205	10.4	59
79	Theoretical realization of two-dimensional M3(C6X6)2 (M = Co, Cr, Cu, Fe, Mn, Ni, Pd, Rh and X = O, S, Se) metal□rganic frameworks. *Applied Materials Today*, **2019**, 15, 405-415	6.6	27
78	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	7.1	35
77	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	7.1	37
76	Band gap and magnetism engineering in Dirac half-metallic Na2C nanosheet via layer thickness, strain and point defects. *Journal of Magnetism and Magnetic Materials*, **2019**, 491, 165565	2.8	26
75	Aromatic molecular junctions between graphene sheets: a molecular dynamics screening for enhanced thermal conductance.. *RSC Advances*, **2019**, 9, 15573-15581	3.7	6
74	Thermal bridging of graphene nanosheets via covalent molecular junctions: A non-equilibrium Green□ function□ensity functional tight-binding study. *Nano Research*, **2019**, 12, 791-799	10	19
73	Theoretical Investigation: 2D N-Graphdiyne Nanosheets as Promising Anode Materials for Li/Na Rechargeable Storage Devices. *ACS Applied Nano Materials*, **2019**, 2, 127-135	5.6	40
72	N-, P-, As-triphenylene-graphdiyne: Strong and stable 2D semiconductors with outstanding capacities as anodes for Li-ion batteries. *Carbon*, **2019**, 141, 291-303	10.4	63
71	2D Hydrogenated graphene-like borophene as a high capacity anode material for improved Li/Na ion batteries: A first principles study. *Materials Today Energy*, **2018**, 8, 22-28	7	58
70	Mechanical responses of two-dimensional MoTe2; pristine 2H, 1T and 1T? and 1T?/2H heterostructure. *Extreme Mechanics Letters*, **2018**, 20, 65-72	3.9	21
69	Borophene hydride: a stiff 2D material with high thermal conductivity and attractive optical and electronic properties. *Nanoscale*, **2018**, 10, 3759-3768	7.7	83
68	Edge-Grafted Molecular Junctions between Graphene Nanoplatelets: Applied Chemistry to Enhance Heat Transfer in Nanomaterials. *Advanced Functional Materials*, **2018**, 28, 1706954	15.6	32
67	Mechanical, optoelectronic and transport properties of single-layer Ca2N and Sr2N electrides. *Journal of Alloys and Compounds*, **2018**, 739, 643-652	5.7	7
66	Carbon ene-yne graphyne monolayer as an outstanding anode material for Li/Na ion batteries. *Applied Materials Today*, **2018**, 10, 115-121	6.6	29
65	Boron Monochalcogenides; Stable and Strong Two-Dimensional Wide Band-Gap Semiconductors. *Energies*, **2018**, 11, 1573	3.1	28
64	N-graphdiyne two-dimensional nanomaterials: Semiconductors with low thermal conductivity and high stretchability. *Carbon*, **2018**, 137, 57-67	10.4	67

63	Boron 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	13	80
62	Anisotropic mechanical properties and strain tuneable band-gap in single-layer SiP, SiAs, GeP and GeAs. *Physica E: Low-Dimensional Systems and Nanostructures*, **2018**, 103, 273-278	3	31
61	Hydrogenation and defect formation control the strength and ductility of MoS2 nanosheets: Reactive molecular dynamics simulation. *Extreme Mechanics Letters*, **2018**, 22, 157-164	3.9	13
60	Lithium halide monolayer sheets: First-principles many-body calculations. *Computational Materials Science*, **2018**, 143, 103-111	3.2	20
59	First-principles investigation of Ag-, Co-, Cr-, Cu-, Fe-, Mn-, Ni-, Pd- and Rh-hexaaminobenzene 2D metal-organic frameworks. *Materials Today Energy*, **2018**, 10, 336-342	7	15
58	Tuning Thermal Transport in C3N Monolayers by Adding and Removing Carbon Atoms. *Physical Review Applied*, **2018**, 10,	4.3	16
57	Anisotropic mechanical and optical response and negative Poisson's ratio in MoC nanomembranes revealed by first-principles simulations. *Nanotechnology*, **2017**, 28, 115705	3.4	41
56	New two-dimensional boron nitride allotropes with attractive electronic and optical properties. *Solid State Communications*, **2017**, 253, 51-56	1.6	29
55	Strong thermal transport along polycrystalline transition metal dichalcogenides revealed by multiscale modeling for MoS2. *Applied Materials Today*, **2017**, 7, 67-76	6.6	29
54	Multiscale modelling of heat conduction in all-MoS2 single-layer heterostructures. *RSC Advances*, **2017**, 7, 11135-11141	3.7	17
53	Electrical and Thermal Transport in Coplanar Polycrystalline Graphene-hBN Heterostructures. *Nano Letters*, **2017**, 17, 1660-1664	11.5	52
52	Flat borophene films as anode materials for Mg, Na or Li-ion batteries with ultra high capacities: A first-principles study. *Applied Materials Today*, **2017**, 8, 60-67	6.6	86
51	Anomalous strain effect on the thermal conductivity of borophene: a reactive molecular dynamics study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2017**, 93, 202-207	3	40
50	Graphene or h-BN paraffin composite structures for the thermal management of Li-ion batteries: A multiscale investigation. *Applied Energy*, **2017**, 202, 323-334	10.7	105
49	Ultra high stiffness and thermal conductivity of graphene like C3N. *Carbon*, **2017**, 118, 25-34	10.4	182
48	Metamorphosis in carbon network: From penta-graphene to biphenylene under uniaxial tension. *FlatChem*, **2017**, 1, 65-73	5.1	24
47	A structural insight into mechanical strength of graphene-like carbon and carbon nitride networks. *Nanotechnology*, **2017**, 28, 055707	3.4	28
46	Record Low Thermal Conductivity of Polycrystalline MoS Films: Tuning the Thermal Conductivity by Grain Orientation. *ACS Applied Materials & Interfaces*, **2017**, 9, 37905-37911	9.5	26

45	Thermal and electronic transport characteristics of highly stretchable graphene kirigami. *Nanoscale*, **2017**, 9, 16329-16341	7.7	19
44	Theoretical realization of Mo2P; a novel stable 2D material with superionic conductivity and attractive optical properties. *Applied Materials Today*, **2017**, 9, 292-299	6.6	32
43	Electronic, optical and thermal properties of highly stretchable 2D carbon Ene-yne graphyne. *Carbon*, **2017**, 123, 344-353	10.4	35
42	Adsorption of Metallic, Metalloidic, and Nonmetallic Adatoms on Two-Dimensional C3N. *Journal of Physical Chemistry C*, **2017**, 121, 18575-18583	3.8	97
41	First-principles investigation of mechanical properties of silicene, germanene and stanene. *Physica E: Low-Dimensional Systems and Nanostructures*, **2017**, 87, 228-232	3	118
40	Mechanical responses of borophene sheets: a first-principles study. *Physical Chemistry Chemical Physics*, **2016**, 18, 27405-27413	3.6	111
39	Borophene as an anode material for Ca, Mg, Na or Li ion storage: A first-principle study. *Journal of Power Sources*, **2016**, 329, 456-461	8.9	147
38	Anisotropic thermal conductivity and mechanical properties of phagraphene: a molecular dynamics study. *RSC Advances*, **2016**, 6, 57773-57779	3.7	53
37	Modeling Kapitza resistance of two-phase composite material. *Composite Structures*, **2016**, 152, 939-946	5.3	41
36	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. *Journal of Power Sources*, **2016**, 307, 657-664	8.9	25
35	Amorphized graphene: A stiff material with low thermal conductivity. *Carbon*, **2016**, 103, 318-326	10.4	70
34	Effect of straining graphene on nanopore creation using Si cluster bombardment: A reactive atomistic investigation. *Journal of Applied Physics*, **2016**, 120, 225108	2.5	7
33	Thermal conductivity and mechanical properties of nitrogenated holey graphene. *Carbon*, **2016**, 106, 1-8	10.4	101
32	Thermal conductivity of MoS 2 polycrystalline nanomembranes. *2D Materials*, **2016**, 3, 035016	5.9	32
31	Mechanical properties of borophene films: a reactive molecular dynamics investigation. *Nanotechnology*, **2016**, 27, 445709	3.4	40
30	Mechanical response of all-MoS2 single-layer heterostructures: a ReaxFF investigation. *Physical Chemistry Chemical Physics*, **2016**, 18, 23695-701	3.6	55
29	Application of silicene, germanene and stanene for Na or Li ion storage: A theoretical investigation. *Electrochimica Acta*, **2016**, 213, 865-870	6.7	171
28	Alignments and network of graphite fillers to improve thermal conductivity of epoxy-based composites. *International Journal of Heat and Mass Transfer*, **2015**, 89, 505-513	4.9	52

27	Modelling heat conduction in polycrystalline hexagonal boron-nitride films. *Scientific Reports*, **2015**, 5, 13228	4.9	90
26	Multiscale modeling of heat conduction in graphene laminates. *Carbon*, **2015**, 85, 1-7	10.4	88
25	Mechanical properties and thermal conductivity of graphitic carbon nitride: A molecular dynamics study. *Computational Materials Science*, **2015**, 99, 285-289	3.2	87
24	Atomistic modeling of mechanical properties of polycrystalline graphene. *Nanotechnology*, **2014**, 25, 215704	3.4	86
23	Multiscale modeling of thermal conductivity of polycrystalline graphene sheets. *Nanoscale*, **2014**, 6, 3344-52	7.7	88
22	Annealing effect on the thermal conductivity of thermoelectric ZnTe nanowires. *Materials Letters*, **2014**, 135, 87-91	3.3	2
21	Mechanical properties of polycrystalline boron-nitride nanosheets. *RSC Advances*, **2014**, 4, 19137-19143	3.7	83
20	Thermal conductivity of ZnTe nanowires. *Journal of Applied Physics*, **2013**, 114, 134314	2.5	15
19	Interphase effect on the elastic and thermal conductivity response of polymer nanocomposite materials: 3D finite element study. *Computational Materials Science*, **2013**, 69, 100-106	3.2	124
18	Thermal conductivity and tensile response of defective graphene: A molecular dynamics study. *Carbon*, **2013**, 63, 460-470	10.4	186
17	Experimental and multiscale modeling of thermal conductivity and elastic properties of PLA/expanded graphite polymer nanocomposites. *Thermochimica Acta*, **2013**, 552, 106-113	2.9	63
16	Combined molecular dynamics-finite element multiscale modeling of thermal conduction in graphene epoxy nanocomposites. *Carbon*, **2013**, 60, 356-365	10.4	115
15	Modeling of two-phase random composite materials by finite element, Mori□Tanaka and strong contrast methods. *Composites Part B: Engineering*, **2013**, 45, 1117-1125	10	114
14	Nitrogen doping and curvature effects on thermal conductivity of graphene: A non-equilibrium molecular dynamics study. *Solid State Communications*, **2012**, 152, 261-264	1.6	90
13	Nitrogen doping and vacancy effects on the mechanical properties of graphene: A molecular dynamics study. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2012**, 376, 1146-1153	2.3	71
12	Investigation of tensile response and thermal conductivity of boron-nitride nanosheets using molecular dynamics simulations. *Physica E: Low-Dimensional Systems and Nanostructures*, **2012**, 44, 1846-1852	3	100
11	Molecular dynamics study on the thermal conductivity and mechanical properties of boron doped graphene. *Solid State Communications*, **2012**, 152, 1503-1507	1.6	75
10	A statistical approach for the evaluation of mechanical properties of silica/epoxy nanocomposite: Verification by experiments. *Computational Materials Science*, **2012**, 59, 108-113	3.2	15

9	Three-dimensional reconstruction and homogenization of heterogeneous materials using statistical correlation functions and FEM. *Computational Materials Science*, **2012**, 51, 372-379	3.2	37
8	Thickness and chirality effects on tensile behavior of few-layer graphene by molecular dynamics simulations. *Computational Materials Science*, **2012**, 53, 298-302	3.2	58
7	A computational and experimental investigation of the mechanical properties of single ZnTe nanowires. *Nanoscale*, **2012**, 4, 897-903	7.7	19
6	Atomistic-Continuum Modeling of the Mechanical Properties of Silica/Epoxy Nanocomposite. *Journal of Engineering Materials and Technology, Transactions of the ASME*, **2012**, 134,	1.8	8
5	Investigation of Mechanical Properties of Silica/Epoxy Nano-Composites by Molecular Dynamics and Finite Element Modeling **2011**, 117-120		
4	Loading Rate Effects on Mechanical Response of Ag, Ni, Al and Cu at Nano-Scale. *Strain*, **2011**, 47, 183-187	1.7	
3	Effective Parameters on the Stress–Strain Curve of Nylon 66/Clay Nanocomposite Using FEM. *Strain* , **2011**, 47, e442-e446	1.7	3
2	Molecular Dynamics Investigation of Loading Rate Effects on Mechanical-Failure Behaviour of FCC Metals. *Journal of Computational and Theoretical Nanoscience*, **2009**, 6, 644-652	0.3	21
1	A Study on the Nanoindentation Behaviour of Single Crystal Silicon Using Hybrid MD-FE Method. *Advanced Materials Research*, **2008**, 32, 259-262	0.5	19