Bohayra Mortazavi

List of Publications by Year
in descending order

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141 papers	7,648 citations	38660 50 h-index	58464 82 g-index
144 all docs	144 docs citations	144 times ranked	5918 citing authors

#	Article	IF	Citations
1	Exceptional piezoelectricity, high thermal conductivity and stiffness and promising photocatalysis in two-dimensional MoSi2N4 family confirmed by first-principles. Nano Energy, 2021, 82, 105716.	8.2	303
2	Application of silicene, germanene and stanene for Na or Li ion storage: A theoretical investigation. Electrochimica Acta, 2016, 213, 865-870.	2.6	245
3	Ultra high stiffness and thermal conductivity of graphene like C3N. Carbon, 2017, 118, 25-34.	5.4	235
4	Thermal conductivity and tensile response of defective graphene: A molecular dynamics study. Carbon, 2013, 63, 460-470.	5.4	229
5	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.	4.0	211
6	First‐Principles Multiscale Modeling of Mechanical Properties in Graphene/Borophene Heterostructures Empowered by Machine‐Learning Interatomic Potentials. Advanced Materials, 2021, 33, e2102807.	11.1	171
7	First-principles investigation of mechanical properties of silicene, germanene and stanene. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 87, 228-232.	1.3	158
8	Mechanical responses of borophene sheets: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 27405-27413.	1.3	149
9	Interphase effect on the elastic and thermal conductivity response of polymer nanocomposite materials: 3D finite element study. Computational Materials Science, 2013, 69, 100-106.	1.4	145
10	Modeling of two-phase random composite materials by finite element, Mori–Tanaka and strong contrast methods. Composites Part B: Engineering, 2013, 45, 1117-1125.	5.9	140
11	Combined molecular dynamics-finite element multiscale modeling of thermal conduction in graphene epoxy nanocomposites. Carbon, 2013, 60, 356-365.	5.4	133
12	Graphene or h-BN paraffin composite structures for the thermal management of Li-ion batteries: A multiscale investigation. Applied Energy, 2017, 202, 323-334.	5.1	133
13	Outstanding strength, optical characteristics and thermal conductivity of graphene-like BC3 and BC6N semiconductors. Carbon, 2019, 149, 733-742.	5.4	126
14	Machine-learning interatomic potentials enable first-principles multiscale modeling of lattice thermal conductivity in graphene/borophene heterostructures. Materials Horizons, 2020, 7, 2359-2367.	6.4	124
15	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.	2.3	122
16	Thermal conductivity and mechanical properties of nitrogenated holey graphene. Carbon, 2016, 106, 1-8.	5.4	118
17	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.	1.3	117
18	Mechanical properties and thermal conductivity of graphitic carbon nitride: A molecular dynamics study. Computational Materials Science, 2015, 99, 285-289.	1.4	112

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19	Adsorption of Metallic, Metalloidic, and Nonmetallic Adatoms on Two-Dimensional C₃N. Journal of Physical Chemistry C, 2017, 121, 18575-18583.	1.5	111
20	Borophene hydride: a stiff 2D material with high thermal conductivity and attractive optical and electronic properties. Nanoscale, 2018, 10, 3759-3768.	2.8	109
21	Accelerating first-principles estimation of thermal conductivity by machine-learning interatomic potentials: A MTP/ShengBTE solution. Computer Physics Communications, 2021, 258, 107583.	3.0	108
22	Modelling heat conduction in polycrystalline hexagonal boron-nitride films. Scientific Reports, 2015, 5, 13228.	1.6	104
23	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
24	Multiscale modeling of heat conduction in graphene laminates. Carbon, 2015, 85, 1-7.	5.4	101
25	Enhancement in hydrogen storage capacities of light metal functionalized Boronâ€“Graphdiyne nanosheets. Carbon, 2019, 147, 199-205.	5.4	100
26	Atomistic modeling of mechanical properties of polycrystalline graphene. Nanotechnology, 2014, 25, 215704.	1.3	99
27	Multiscale modeling of thermal conductivity of polycrystalline graphene sheets. Nanoscale, 2014, 6, 3344-3352.	2.8	98
28	Nitrogen doping and curvature effects on thermal conductivity of graphene: A non-equilibrium molecular dynamics study. Solid State Communications, 2012, 152, 261-264.	0.9	97
29	Exploring phononic properties of two-dimensional materials using machine learning interatomic potentials. Applied Materials Today, 2020, 20, 100685.	2.3	96
30	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.	2.5	93
31	Mechanical properties of polycrystalline boron-nitride nanosheets. RSC Advances, 2014, 4, 19137-19143.	1.7	90
32	Molecular dynamics study on the thermal conductivity and mechanical properties of boron doped graphene. Solid State Communications, 2012, 152, 1503-1507.	0.9	89
33	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.	9.5	84
34	Amorphized graphene: A stiff material with low thermal conductivity. Carbon, 2016, 103, 318-326.	5.4	82
35	N-graphdiyne two-dimensional nanomaterials: Semiconductors with low thermal conductivity and high stretchability. Carbon, 2018, 137, 57-67.	5.4	82
36	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.	0.9	79

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37	Experimental and multiscale modeling of thermal conductivity and elastic properties of PLA/expanded graphite polymer nanocomposites. Thermochimica Acta, 2013, 552, 106-113.	1.2	74
38	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
39	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
40	Thickness and chirality effects on tensile behavior of few-layer graphene by molecular dynamics simulations. Computational Materials Science, 2012, 53, 298-302.	1.4	70
41	Anisotropic thermal conductivity and mechanical properties of phagraphene: a molecular dynamics study. RSC Advances, 2016, 6, 57773-57779.	1.7	68
42	Mechanical response of all-MoS₂ single-layer heterostructures: a ReaxFF investigation. Physical Chemistry Chemical Physics, 2016, 18, 23695-23701.	1.3	67
43	Electrical and Thermal Transport in Coplanar Polycrystalline Grapheneâ€“hBN Heterostructures. Nano Letters, 2017, 17, 1660-1664.	4.5	62
44	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.	2.5	61
45	Tunable electronic and magnetic properties of graphene/carbon-nitride van der Waals heterostructures. Applied Surface Science, 2020, 505, 144450.	3.1	61
46	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
47	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
48	Theoretical Investigation: 2D N-Graphdiyne Nanosheets as Promising Anode Materials for Li/Na Rechargeable Storage Devices. ACS Applied Nano Materials, 2019, 2, 127-135.	2.4	56
49	Intelligent on-demand design of phononic metamaterials. Nanophotonics, 2022, 11, 439-460.	2.9	55
50	Modeling Kapitza resistance of two-phase composite material. Composite Structures, 2016, 152, 939-946.	3.1	53
51	New two-dimensional boron nitride allotropes with attractive electronic and optical properties. Solid State Communications, 2017, 253, 51-56.	0.9	53
52	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.	1.3	51
53	Mechanical properties of borophene films: a reactive molecular dynamics investigation. Nanotechnology, 2016, 27, 445709.	1.3	50
54	First-principles investigation of mechanical, electronic and optical properties of H-, F- and Cl-diamane. Applied Surface Science, 2020, 528, 147035.	3.1	47

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55	Metamorphosis in carbon network: From penta-graphene to biphenylene under uniaxial tension. FlatChem, 2017, 1, 65-73.	2.8	46
56	Electronic, optical and thermal properties of highly stretchable 2D carbon Ene-yne graphyne. Carbon, 2017, 123, 344-353.	5.4	46
57	Nanoporous graphene: A 2D semiconductor with anisotropic mechanical, optical and thermal conduction properties. Carbon, 2019, 147, 377-384.	5.4	46
58	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.	1.3	45
59	As₂S₃, As₂Se₃ and As₂Te₃ nanosheets: superstretchable semiconductors with anisotropic carrier mobilities and optical properties. Journal of Materials Chemistry C, 2020, 8, 2400-2410.	2.7	45
60	Carbon ene-yne graphyne monolayer as an outstanding anode material for Li/Na ion batteries. Applied Materials Today, 2018, 10, 115-121.	2.3	44
61	Ab initio prediction of semiconductivity in a novel two-dimensional Sb2X3 (X= S, Se, Te) monolayers with orthorhombic structure. Scientific Reports, 2021, 11, 10366.	1.6	44
62	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
63	Three-dimensional reconstruction and homogenization of heterogeneous materials using statistical correlation functions and FEM. Computational Materials Science, 2012, 51, 372-379.	1.4	41
64	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
65	Machine learning assisted multiscale modeling of composite phase change materials for Li-ion batteriesâ€™ thermal management. International Journal of Heat and Mass Transfer, 2021, 172, 121199.	2.5	41
66	Edgeâ€Grafted Molecular Junctions between Graphene Nanoplatelets: Applied Chemistry to Enhance Heat Transfer in Nanomaterials. Advanced Functional Materials, 2018, 28, 1706954.	7.8	39
67	High thermal conductivity in semiconducting Janus and non-Janus diamanes. Carbon, 2020, 167, 51-61.	5.4	39
68	Embedding of atoms into the nanopore sites of the C₆N₆ and C₆N₈ porous carbon nitride monolayers with tunable electronic properties. Physical Chemistry Chemical Physics, 2020, 22, 6418-6433.	1.3	38
69	Ultrahigh thermal conductivity and strength in direct-gap semiconducting graphene-like BC6N: A first-principles and classical investigation. Carbon, 2021, 182, 373-383.	5.4	38
70	Thermal conductivity of MoS ₂ polycrystalline nanomembranes. 2D Materials, 2016, 3, 035016.	2.0	37
71	Theoretical realization of two-dimensional M3(C6X6)2 (M = Co, Cr, Cu, Fe, Mn, Ni, Pd, Rh and X = O, S,) Tj ETQq1 1 0.784314 rgBT /O	2.3	37
72	Strong thermal transport along polycrystalline transition metal dichalcogenides revealed by multiscale modeling for MoS 2. Applied Materials Today, 2017, 7, 67-76.	2.3	35

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73	Record Low Thermal Conductivity of Polycrystalline MoS₂ Films: Tuning the Thermal Conductivity by Grain Orientation. ACS Applied Materials & Interfaces, 2017, 9, 37905-37911.	4.0	35
74	Mechanical responses of two-dimensional MoTe2; pristine 2H, 1T and 1Tâ€² and 1Tâ€²/2H heterostructure. Extreme Mechanics Letters, 2018, 20, 65-72.	2.0	34
75	A machine-learning-based investigation on the mechanical/failure response and thermal conductivity of semiconducting BC2N monolayers. Carbon, 2022, 188, 431-441.	5.4	34
76	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.	2.5	33
77	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.	4.0	32
78	A structural insight into mechanical strength of graphene-like carbon and carbon nitride networks. Nanotechnology, 2017, 28, 055707.	1.3	32
79	Boron Monochalcogenides; Stable and Strong Two-Dimensional Wide Band-Gap Semiconductors. Energies, 2018, 11, 1573.	1.6	32
80	Two-Dimensional SiP, SiAs, GeP and GeAs as Promising Candidates for Photocatalytic Applications. Coatings, 2019, 9, 522.	1.2	32
81	Efficient machine-learning based interatomic potentialsfor exploring thermal conductivity in two-dimensional materials. JPhys Materials, 2020, 3, 02LT02.	1.8	32
82	Exploring thermal expansion of carbon-based nanosheets by machine-learning interatomic potentials. Carbon, 2022, 186, 501-508.	5.4	30
83	Two-dimensional PdPS and PdPSe nanosheets: Novel promising sensing platforms for harmful gas molecules. Applied Surface Science, 2022, 579, 152115.	3.1	30
84	Thermal bridging of graphene nanosheets via covalent molecular junctions: A non-equilibrium Greenâ€™s functionsâ€“density functional tight-binding study. Nano Research, 2019, 12, 791-799.	5.8	29
85	Thermal and electronic transport characteristics of highly stretchable graphene kirigami. Nanoscale, 2017, 9, 16329-16341.	2.8	28
86	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.	1.0	27
87	Lithium halide monolayer sheets: First-principles many-body calculations. Computational Materials Science, 2018, 143, 103-111.	1.4	26
88	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.	1.5	26
89	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
90	Tuning Thermal Transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> Monolayers by Adding and Removing Carbon Atoms. Physical Review Applied, 2018, 10, .	1.5	25

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91	High tensile strength and thermal conductivity in BeO monolayer: A first-principles study. FlatChem, 2021, 28, 100257.	2.8	24
92	Anisotropic mechanical response, high negative thermal expansion, and outstanding dynamical stability of biphenylene monolayer revealed by machine-learning interatomic potentials. FlatChem, 2022, 32, 100347.	2.8	24
93	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.	5.4	24
94	Ultrahigh stiffness and anisotropic Dirac cones in BeN4 and MgN4 monolayers: a first-principles study. Materials Today Nano, 2021, 15, 100125.	2.3	23
95	Mechanical, optical, and thermoelectric properties of semiconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>ZnIn</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>		

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109	First-principles investigation of electronic, optical, mechanical and heat transport properties of pentadiamond: A comparison with diamond. Carbon Trends, 2021, 3, 100036.	1.4	16
110	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.	1.3	16
111	Effect of straining graphene on nanopore creation using Si cluster bombardment: A reactive atomistic investigation. Journal of Applied Physics, 2016, 120, .	1.1	15
112	Electronic, optical and thermoelectric properties of boron-doped nitrogenated holey graphene. Physical Chemistry Chemical Physics, 2020, 22, 21147-21157.	1.3	15
113	Mechanical, optoelectronic and transport properties of single-layer Ca2N and Sr2N electrides. Journal of Alloys and Compounds, 2018, 739, 643-652.	2.8	14
114	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
115	Exploring tensile piezoelectricity and bending flexoelectricity of diamane monolayers by machine learning. Carbon, 2021, 185, 558-567.	5.4	13
116	Anisotropic charge transport in 1D and 2D BeN4 and MgN4 nanomaterials: A first-principles study. FlatChem, 2022, 31, 100327.	2.8	13
117	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.	1.3	10
118	Exploration of mechanical, thermal conductivity and electromechanical properties of graphene nanoribbon springs. Nanoscale Advances, 2020, 2, 3394-3403.	2.2	9
119	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.	3.1	9
120	Exploring the mechanical properties of two-dimensional carbon-nitride polymer nanocomposites by molecular dynamics simulations. Composite Structures, 2022, 281, 115004.	3.1	9
121	Atomistic-Continuum Modeling of the Mechanical Properties of Silica/Epoxy Nanocomposite. Journal of Engineering Materials and Technology, Transactions of the ASME, 2012, 134, .	0.8	8
122	Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>7</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math> : Room-temperature excitons with large binding energies and high thermal conductivities. Physical Review Materials, 2020, 4, .	0.9	8
123	Aromatic molecular junctions between graphene sheets: a molecular dynamics screening for enhanced thermal conductance. RSC Advances, 2019, 9, 15573-15581.	1.7	7
124	Highly anisotropic mechanical and optical properties of 2D NbOX2 (XÂ=ÂCl, Br, I) revealed by first-principle. Nanotechnology, 2022, 33, 275701.	1.3	7
125	A Multiscale Investigation on the Thermal Transport in Polydimethylsiloxane Nanocomposites: Graphene vs. Borophene. Nanomaterials, 2021, 11, 1252.	1.9	6
126	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.	1.1	6

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127	Monoelemental two-dimensional iodinene nanosheets: a first-principles study of the electronic and optical properties. Journal Physics D: Applied Physics, 2022, 55, 135104.	1.3	5
128	Effective Parameters on the Stressâ€“Strain Curve of Nylon 66/Clay Nanocomposite Using FEM. Strain, 2011, 47, e442.	1.4	4
129	Predicting the Electronic and Structural Properties of Two-Dimensional Materials Using Machine Learning. Computers, Materials and Continua, 2021, 67, 1287-1300.	1.5	3
130	Molecular Dynamics Modeling of Mechanical Properties of Polymer Nanocomposites Reinforced by C7N6 Nanosheet. Surfaces, 2021, 4, 240-254.	1.0	3
131	Annealing effect on the thermal conductivity of thermoelectric ZnTe nanowires. Materials Letters, 2014, 135, 87-91.	1.3	2
132	Molecular Junctions Enhancing Thermal Transport within Graphene Polymer Nanocomposite: A Molecular Dynamics Study. Nanomaterials, 2021, 11, 2480.	1.9	2
133	Molecular Dynamics Investigation of Î²-SiC Behavior Under Three-Axial Tensile Loading. Journal of Computational and Theoretical Nanoscience, 2011, 8, 2187-2192.	0.4	1
134	A Study on the Uniaxial Tension of FCC Metals at Nano Level Using MD. Advanced Materials Research, 0, , 255-258.	0.3	1
135	A Study on the Nanoindentation Behaviour of Single Crystal Silicon Using Hybrid MD-FE Method. Advanced Materials Research, 0, , 259-262.	0.3	1
136	Comment on â€˜MoSi2N4 single-layer: a novel two-dimensional material with outstanding mechanical, thermal, electronic and optical propertiesâ€™. Journal Physics D: Applied Physics, 2022, 55, 068001.	1.3	1
137	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
138	Loading Rate Effects on Mechanical Response of Ag, Ni, Al and Cu at Nanoâ€Scale. Strain, 2011, 47, 183-187.	1.4	0
139	Comment on â€œTwo-dimensional carbon nitride C6N nanosheet with egg-comb-like structure and electronic properties of a semimetal [Nanotechnology 2021, 32, 215702]â€. Nanotechnology, 2022, , .	1.3	0
140	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
141	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.	1.1	0