Keivan Esfarjani

List of Publications by Year
in descending order

153 papers	10,275 citations	50170 46 h-index	32761 100 g-index
155 all docs	155 docs citations	155 times ranked	8522 citing authors

#	Article	IF	Citations
1	Perspectives on thermoelectrics: from fundamentals to device applications. Energy and Environmental Science, 2012, 5, 5147-5162.	15.6	1,080
2	High thermoelectric performance by resonant dopant indium in nanostructured SnTe. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13261-13266.	3.3	632
3	Heat transport in silicon from first-principles calculations. Physical Review B, 2011, 84, .	1.1	618
4	Coherent Phonon Heat Conduction in Superlattices. Science, 2012, 338, 936-939.	6.0	489
5	Resonant bonding leads to low lattice thermal conductivity. Nature Communications, 2014, 5, 3525.	5.8	484
6	Phonon conduction in PbSe, PbTe, and PbTe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>from first-principles calculations. Physical Review B, 2012, 85, .	1.1	463
7	Thermal Conductivity Spectroscopy Technique to Measure Phonon Mean Free Paths. Physical Review Letters, 2011, 107, 095901.	2.9	438
8	Enhancement of thermoelectric figure-of-merit by resonant states of aluminium doping in lead selenide. Energy and Environmental Science, 2012, 5, 5246-5251.	15.6	372
9	Method to extract anharmonic force constants from first principles calculations. Physical Review B, 2008, 77, .	1.1	295
10	Hydrodynamic phonon transport in suspended graphene. Nature Communications, 2015, 6, 6290.	5.8	254
11	Stronger phonon scattering by larger differences in atomic mass and size in p-type half-Heuslers Hf1â^'xTixCoSb0.8Sn0.2. Energy and Environmental Science, 2012, 5, 7543.	15.6	244
12	Enhancing phonon transmission across a Si/Ge interface by atomic roughness: First-principles study with the Green's function method. Physical Review B, 2012, 86, .	1.1	232
13	Significant Reduction of Lattice Thermal Conductivity by the Electron-Phonon Interaction in Silicon with High Carrier Concentrations: A First-Principles Study. Physical Review Letters, 2015, 114, 115901.	2.9	229
14	Thermal conductivity of half-Heusler compounds from first-principles calculations. Physical Review B, 2011, 84, .	1.1	187
15	Insights into exfoliation possibility of MAX phases to MXenes. Physical Chemistry Chemical Physics, 2018, 20, 8579-8592.	1.3	182
16	On the importance of optical phonons to thermal conductivity in nanostructures. Applied Physics Letters, 2011, 99, .	1.5	137
17	Spin and band-gap engineering in doped graphene nanoribbons. Physical Review B, 2008, 78, .	1.1	128
18	Thermal interface conductance in Si/Ge superlattices by equilibrium molecular dynamics. Physical Review B, 2012, 85, .	1.1	128

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19	Nonlinear Coherent Transport Through Doped Nanotube Junctions. Physical Review Letters, 1999, 82, 5084-5087.	2.9	124
20	Effect of nanoparticle scattering on thermoelectric power factor. Applied Physics Letters, 2009, 94, 202105.	1.5	124
21	Novel MAB phases and insights into their exfoliation into 2D MBenes. Nanoscale, 2019, 11, 11305-11314.	2.8	120
22	Thermoelectric properties of a nanocontact made of two-capped single-wall carbon nanotubes calculated within the tight-binding approximation. Physical Review B, 2006, 73, .	1.1	117
23	Microscopic mechanism of low thermal conductivity in lead telluride. Physical Review B, 2012, 85, .	1.1	115
24	Study of the Thermoelectric Properties of Lead Selenide Doped with Boron, Gallium, Indium, or Thallium. Journal of the American Chemical Society, 2012, 134, 17731-17738.	6.6	105
25	Electronic and transport properties of N-P doped nanotubes. Applied Physics Letters, 1999, 74, 79-81.	1.5	100
26	Gallium arsenide thermal conductivity and optical phonon relaxation times from first-principles calculations. Europhysics Letters, 2013, 101, 16001.	0.7	100
27	Transition from near-field thermal radiation to phonon heat conduction at sub-nanometre gaps. Nature Communications, 2015, 6, 6755.	5.8	95
28	Cluster scattering effects on phonon conduction in graphene. Physical Review B, 2010, 81, .	1.1	93
29	Molecular dynamics simulation of thermal energy transport in polydimethylsiloxane. Journal of Applied Physics, 2011, 109, .	1.1	87
30	Ab InitioMolecular Dynamics Simulations for Collision betweenC60â^'and Alkali-Metal Ions: A Possibility of Li@C60. Physical Review Letters, 1996, 76, 3590-3593.	2.9	85
31	Computational Materials Science. Springer Series in Solid-state Sciences, 1999, , .	0.3	85
32	Thermal Interface Conductance Between Aluminum and Silicon by Molecular Dynamics Simulations. Journal of Computational and Theoretical Nanoscience, 2015, 12, 168-174.	0.4	78
33	Ab initio optimization of phonon drag effect for lower-temperature thermoelectric energy conversion. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14777-14782.	3.3	75
34	Site Occupation Reversal in theFeâ^'CrÏƒPhase. Physical Review Letters, 1995, 75, 3142-3145.	2.9	72
35	Semi-metals as potential thermoelectric materials. Scientific Reports, 2018, 8, 9876.	1.6	71
36	Vibrational modes and IR analysis of neutral photopolymerizedC60dimers. Physical Review B, 1998, 57, 223-229.	1.1	62

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37	Enhancing the Thermoelectric Power Factor by Using Invisible Dopants. Advanced Materials, 2013, 25, 1577-1582.	11.1	61
38	Green's function studies of phonon transport across Si/Ge superlattices. Physical Review B, 2014, 89, .	1.1	60
39	Cloaking Core-Shell Nanoparticles from Conducting Electrons in Solids. Physical Review Letters, 2012, 109, 126806.	2.9	58
40	Non-diffusive relaxation of a transient thermal grating analyzed with the Boltzmann transport equation. Journal of Applied Physics, 2013, 114, 104302.	1.1	58
41	Low-Temperature Thermoelectric Power Factor Enhancement by Controlling Nanoparticle Size Distribution. Nano Letters, 2011, 11, 225-230.	4.5	56
42	Localization-delocalization transition in a one one-dimensional system with long-range correlated off-diagonal disorder. Physical Review B, 2005, 72, .	1.1	55
43	Lattice thermal conductivity of Bi, Sb, and Bi-Sb alloy from first principles. Physical Review B, 2014, 89, .	1.1	55
44	Band structure and chemical bonding inC58BN heterofullerenes. Physical Review B, 1994, 50, 17830-17836.	1.1	53
45	Spin filtering and spin diode devices in quantum wire systems. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 27, 325-331.	1.3	51
46	Thermal management and non-reciprocal control of phonon flow via optomechanics. Nature Communications, 2018, 9, 1207.	5.8	48
47	Thermoelectric properties of semimetals. Physical Review Materials, 2019, 3, .	0.9	47
48	Ab Initio study of dopant insertion into carbon nanotubes. Journal of Chemical Physics, 1999, 111, 2164-2168.	1.2	44
49	Nonlinear Peltier effect in semiconductors. Applied Physics Letters, 2007, 91, 122104.	1.5	44
50	Temperature-dependent thermal conductivity in silicon nanostructured materials studied by the Boltzmann transport equation. Physical Review B, 2016, 93, .	1.1	44
51	Unexpectedly high cross-plane thermoelectric performance of layered carbon nitrides. Journal of Materials Chemistry A, 2019, 7, 2114-2121.	5.2	44
52	Solidification of the two-dimensional electron gas in high magnetic fields. Physical Review B, 1990, 42, 10758-10760.	1.1	42
53	A Mechanism for Quantum Melting in Two Dimensions. Europhysics Letters, 1991, 14, 361-365.	0.7	42
54	Thermoelectric transport perpendicular to thin-film heterostructures calculated using the Monte Carlo technique. Physical Review B, 2006, 74, .	1.1	42

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55	Negative differential resistance in molecular junctions: Application to graphene ribbon junctions. Physical Review B, 2008, 78, .	1.1	42
56	Lifetime of sub-THz coherent acoustic phonons in a GaAs-AlAs superlattice. Applied Physics Letters, 2013, 102, .	1.5	41
57	Self-consistent tight-binding formalism for charged systems. Journal of Physics Condensed Matter, 1998, 10, 8257-8267.	0.7	39
58	Importance of local force fields on lattice thermal conductivity reduction in PbTe 1âˆ’x Se x alloys. Europhysics Letters, 2013, 102, 46002.	0.7	39
59	Finite-temperature transport of a pinned 2D electron lattice. Physical Review Letters, 1991, 66, 652-654.	2.9	33
60	First principles calculations of solid-state thermionic transport in layered van der Waals heterostructures. Nanoscale, 2016, 8, 14695-14704.	2.8	33
61	Effect of Nanoparticles on Electron and Thermoelectric Transport. Journal of Electronic Materials, 2009, 38, 954-959.	1.0	32
62	Isotropic and energy-selective electron cloaks on graphene. Physical Review B, 2013, 88, .	1.1	30
63	Disorder, screening, and quantum Hall oscillations. Physical Review B, 1990, 41, 1042-1053.	1.1	29
64	Many-electron states of nitrogen-vacancy centers in diamond and spin density calculations. Physical Review B, 2011, 84, .	1.1	27
65	Improved Thermoelectric Performance of Ecoâ€Friendly Î²â€FeSi 2 â€“SiGe Nanocomposite via Synergistic Hierarchical Structuring, Phase Percolation, and Selective Doping. Advanced Functional Materials, 2019, 29, 1903157.	7.8	27
66	Cross-Plane Seebeck Coefficient Measurement of Misfit Layered Compounds (SnSe)_n(TiSe₂)_n (n = 1,3,4,5). Nano Letters, 2017, 17, 1978-1986.	4.5	25
67	Evidence for pseudoâ€“Jahn-Teller distortions in the charge density wave phase of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>-</mml:mtext>â”‚ Physical Review B, 2020, 101, .	1.1	25
68	Analytical results on coherent conductance in a general periodic quantum dot: Transfer matrix method. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 28, 150-161.	1.3	23
69	Monte Carlo simulation of electron transport in degenerate and inhomogeneous semiconductors. Applied Physics Letters, 2007, 90, 092111.	1.5	23
70	First-principles study of thermal transport inFeSb2. Physical Review B, 2014, 89, .	1.1	23
71	The thermal and mechanical properties of hafnium orthosilicate: Experiments and first-principles calculations. Materialia, 2020, 12, 100793.	1.3	23
72	Finite-temperature two-dimensional Wigner transition. Physical Review B, 1991, 44, 11498-11501.	1.1	22

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73	Client-server model of integrated production facilities. International Journal of Production Research, 1998, 36, 3295-3321.	4.9	22
74	In-situ infrared spectroscopy of a photoirradiated potassium-doped C60 film. Chemical Physics Letters, 1999, 315, 19-24.	1.2	22
75	Non-linear enhancement of thermoelectric performance of a TiSe₂ monolayer due to tensile strain, from first-principles calculations. Journal of Materials Chemistry C, 2019, 7, 7308-7317.	2.7	22
76	Phonon scattering effects from point and extended defects on thermal conductivity studied via ion irradiation of crystals with self-impurities. Physical Review Materials, 2018, 2, .	0.9	22
77	Effect of filler mass and binding on thermal conductivity of fully filled skutterudites. Physical Review B, 2010, 82, .	1.1	21
78	High-Performance Solid-State Thermionic Energy Conversion Based on 2D van der Waals Heterostructures: A First-Principles Study. Scientific Reports, 2018, 8, 9303.	1.6	21
79	Some analytical results in phase coherent transport in quantum wire. Physica E: Low-Dimensional Systems and Nanostructures, 2004, 25, 119-130.	1.3	20
80	A bilayer of Wigner crystal in the harmonic approximation. Journal of Physics Condensed Matter, 1995, 7, 7217-7226.	0.7	18
81	Self-consistent phonon and magnetophonon and cubic anharmonic corrections of the 2D electron lattice. Journal of Physics Condensed Matter, 1991, 3, 5825-5836.	0.7	17
82	MODELING HEAT CONDUCTION FROM FIRST PRINCIPLES. Annual Review of Heat Transfer, 2014, 17, 9-47.	0.3	17
83	Ab Initio Computer Simulations on Microclusters: Structures and Electronic Properties. Springer Series in Cluster Physics, 2002, , 9-88.	0.3	16
84	Coherent conductance in an alternating dot: exact results. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 27, 227-234.	1.3	15
85	Interfacial Water Facilitates Energy Transfer by Inducing Extended Vibrations in Membrane Lipids. Journal of Physical Chemistry B, 2012, 116, 6455-6460.	1.2	15
86	Molecular Dynamics Study of Cubic Boron Nitride Nanoparticles: Decomposition with Phase Segregation during Melting. ACS Nano, 2016, 10, 10563-10572.	7.3	15
87	Effect of orientation on the band structure of C58BN hetero-fullerenes in fcc solid phase. Solid State Communications, 1996, 97, 539-542.	0.9	12
88	Dislocation waves in a two-dimensional Coulomb lattice. Physical Review B, 1992, 46, 4638-4643.	1.1	11
89	High-pressure phases of hydrogen cyanide: formation of hydrogenated carbon nitride polymers and layers and their electronic properties. Journal of Physics Condensed Matter, 2011, 23, 405403.	0.7	11
90	Lattice relaxation in many-electron states of the diamond vacancy. Physical Review B, 2005, 71, .	1.1	10

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91	Molecular dynamics of single wall carbon nanotube growth on nickel surface. Computational Materials Science, 2006, 36, 117-120.	1.4	10
92	First-Principles Calculation of Charge Transfer at the Siliconâ€“Organic Interface. Journal of Physical Chemistry C, 2017, 121, 15529-15537.	1.5	10
93	Screening at doped nanotube junctions beyond linear response. Physical Review B, 2002, 65, .	1.1	9
94	Details of a theoretical model for electronic structure of the diamond vacancies. Diamond and Related Materials, 2004, 13, 2125-2130.	1.8	9
95	An ab initio study of multiple phonon scattering resonances in silicon germanium alloys. Journal of Applied Physics, 2015, 117, 174301.	1.1	9
96	In Situ FTIR, XPS, and STM Studies of the Nano-Structure of a Photopolymerized C₆₀ Film. Molecular Crystals and Liquid Crystals, 2000, 340, 689-694.	0.3	8
97	Analytical results on ballistic transport in a periodic molecular wire. Chemical Physics, 2005, 317, 43-48.	0.9	8
98	First principles molecular dynamics studies of elastic constants, ideal tensile strength, chemistry of crack initiation, and surface and cohesive energies in amorphous silicon. Philosophical Magazine, 2014, 94, 2913-2936.	0.7	8
99	Thermomagnetic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> single crystal in the temperature range from 55ÂK to 380 K. Physical Review Materials, 2021, 5, .	2.9	8
100	Nernst coefficient within relaxation time approximation. Physical Review B, 2021, 103, .	1.1	8
101	Shear modulus of the magnetophonon wave function. Solid State Communications, 1991, 79, 387-388.	0.9	7
102	ELECTRONIC PROPERTIES OF C58BN HETEROFULLERENES. Surface Review and Letters, 1996, 03, 747-752.	0.5	7
103	The Nanostructure of C60 Photopolymers. Springer Series in Cluster Physics, 2002, , 135-169.	0.3	7
104	Oscillator strength calculations in color centers of diamond and the role of spin. European Physical Journal B, 2004, 39, 441-446.	0.6	6
105	Spin dynamics characterization in magnetic dots. Physica B: Condensed Matter, 2007, 399, 81-93.	1.3	6
106	Strain-induced instability of spherical nanodiamond hydrocarbons: Effect of surface<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CH</mml:mtext></mml:mrow><mml:mi>n</mml:mi></mml:msub> charging. Physical Review B, 2009, 79, .	1.1	6
107	Abundance of Nanoclusters in a Molecular Beam: The Magic Numbers for Lennard-Jones Potential. Journal of Cluster Science, 2015, 26, 473-490.	1.7	6
108	Ultra-high lattice thermal conductivity and the effect of pressure in superhard hexagonal BC₂N. Journal of Materials Chemistry C, 2020, 8, 15705-15716.	2.7	6

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109	Effect of exchange-correlation functional type and spin-orbit coupling on thermoelectric properties of ZrTe2. Journal of Solid State Chemistry, 2021, 302, 122414.	1.4	6
110	Tight-binding parametrization of transition metal elements from LCAO ab initio Hamiltonians. Computational Materials Science, 1998, 9, 343-347.	1.4	5
111	Ab Initio Methods. Springer Series in Solid-state Sciences, 1999, , 7-138.	0.3	5
112	An All-electron First-principles Molecular Dynamics Method and a Possibility of its Application to Atomistically Distorted Systems. Advances in Materials Research, 1998, , 210-219.	0.2	5
113	Realization of an effective ultrahigh magnetic field on a nanoscale. Journal of Physics Condensed Matter, 2001, 13, L49-L55.	0.7	4
114	Electronic properties of magnetically doped nanotubes. Bulletin of Materials Science, 2003, 26, 105-107.	0.8	4
115	Calculation of thermomagnetic properties using first-principles density functional theory. Computational Materials Science, 2022, 210, 111412.	1.4	4
116	Stability and vibrational spectra of toroidal isomers of C_{240}. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 41, 73-76.	1.0	3
117	The three-fermion problem in two and three dimensions; a unified variational approach. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 749-756.	0.6	3
118	Localized basis set optimization. Computational Materials Science, 1999, 15, 351-356.	1.4	3
119	Why the all-electron full-potential approach is suitable for calculations on fullerenes and nanotubes?. Journal of Molecular Graphics and Modelling, 2001, 19, 270-273.	1.3	3
120	Transport properties of a nanotube-based transistor. European Physical Journal D, 2001, 16, 353-355.	0.6	3
121	Nonlinear Charging and Transport Times in Doped Nanotubes Junctions. Journal of the Physical Society of Japan, 2005, 74, 515-518.	0.7	3
122	Enhanced Cooling in Doped Semiconductors Due to Nonlinear Peltier Effect. Materials Research Society Symposia Proceedings, 2007, 1044, 1.	0.1	3
123	Gap tuning and effective electron correlation energy in amorphous silicon: A first principles density functional theory-based molecular dynamics study. Computational Materials Science, 2015, 102, 110-118.	1.4	3
124	Tunable lattice distortion in MgCoNiCuZnO5 entropy-stabilized oxide. Journal of Materials Research, 2021, 36, 1615-1623.	1.2	3
125	Electronic, Transport and Mechanical Properties of Carbon Nanotubes. Springer Series in Cluster Physics, 2002, , 187-220.	0.3	3
126	Fourier transform infrared and mass spectrometry studies of a photoirradiated KxC60 film. European Physical Journal D, 1999, 9, 363-367.	0.6	2

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127	Relationship between lattice relaxation and electron delocalization in diamond vacancies. Physica B: Condensed Matter, 2006, 376-377, 324-326.	1.3	2
128	GROUND-STATE ENERGY AND COMPRESSIBILITY OF A DISORDERED TWO-DIMENSIONAL ELECTRON GAS. International Journal of Modern Physics B, 2007, 21, 2134-2144.	1.0	2
129	Ab Initio Methods. , 2018, , 7-197.		2
130	Low-resistance contact in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoSe</mml:mi><mml:mn>2</mml:mn></mml:msub></m -based solid-state thermionic devices. Physical Review B, 2022, 105, .	1.1	2
131	Electron-interaction effects on transport characteristics of nanotubes. Physica B: Condensed Matter, 2002, 323, 242-243.	1.3	1
132	Statics and dynamics of phase segregation in multicomponent fermion gas. European Physical Journal D, 2002, 21, 181-189.	0.6	1
133	Properties of charge and magnetic impurities in a spin-polarized electron gas: A semiclassical approach. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 28, 313-322.	1.3	1
134	Generalized Hubbard model for many-electron states of the diamond vacancies: A non-CI approach. Physica Status Solidi (B): Basic Research, 2006, 243, 1269-1275.	0.7	1
135	Metallic Composites Phase-Change Materials for High-Temperature Thermal Energy Storage. , 2013, , .		1
136	Theory of Non-Equilibrium Heat Transport in Anharmonic Multiprobe Systems at High Temperatures. Entropy, 2021, 23, 1630.	1.1	1
137	Electronic Properties of C58Bn Fullerenes. Materials Research Society Symposia Proceedings, 1994, 349, 225.	0.1	0
138	Search for the Ground State of C60B10. Materials Research Society Symposia Proceedings, 1994, 359, 229.	0.1	0
139	Phase Stability of the Sigma Phase in Fe-Cr Based Alloys. Materials Research Society Symposia Proceedings, 1995, 408, 369.	0.1	0
140	Molecular dynamics simulation on aligning process of C[sub 60] on various substrates and the origin of specific surface electronic states. , 1997, , .		0
141	Simulated annealing of small silicon clusters by tight-binding. , 1997, , .		0
142	Tight-Binding Methods. Springer Series in Solid-state Sciences, 1999, , 139-170.	0.3	0
143	Charge oscillation at doped nanotube junctions. AIP Conference Proceedings, 2001, , .	0.3	0
144	Spin valve effect in magnetically doped nanotube-based transistors. AIP Conference Proceedings, 2001, , .	0.3	0

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145	Effect of Elastic Interaction on Self-Assembled Island Spatial Arrangement. Materials Transactions, 2001, 42, 2279-2282.	0.4	0
146	Thermal Conductivity of Cage-Like Structures. , 2011, , .		0
147	Delocalization of phonons and energy spectrum in disordered nonlinear systems. Physical Review B, 2020, 101, .	1.1	0
148	Effect of inter-island interaction on the growth of self-assembled quantum dots. Springer Proceedings in Physics, 2001, , 389-390.	0.1	0
149	GROUND-STATE ENERGY AND COMPRESSIBILITY OF A DISORDERED TWO-DIMENSIONAL ELECTRON GAS. , 2007, , .		0
150	First-Principles-Based Interatomic Potential for SI and Its Thermal Conductivity. , 2011, , .		0
151	Fourier transform infrared and mass spectrometry studies of a photoirradiated KxC60 film. , 1999, , 363-367.		0
152	Tight-Binding Methods. , 2018, , 199-230.		0
153	Ab initio phonon transport across grain boundaries in graphene using machine learning based on small dataset. Physical Review Materials, 2022, 6, .	0.9	0