Qing-Xia Pei

List of Publications by Year
in descending order

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119 papers	5,539 citations	71102 41 h-index	88630 70 g-index
119 all docs	119 docs citations	119 times ranked	5030 citing authors

#	Article	IF	Citations
1	A molecular dynamics study of the mechanical properties of hydrogen functionalized graphene. Carbon, 2010, 48, 898-904.	10.3	442
2	Mechanical properties of graphynes under tension: A molecular dynamics study. Applied Physics Letters, 2012, 101, 081909.	3.3	217
3	A theoretical analysis of the thermal conductivity of hydrogenated graphene. Carbon, 2011, 49, 4752-4759.	10.3	176
4	Phonon thermal conductivity of monolayer MoS₂ sheet and nanoribbons. Applied Physics Letters, 2013, 103, 133113.	3.3	167
5	Manipulating the Thermal Conductivity of Monolayer MoS₂ via Lattice Defect and Strain Engineering. Journal of Physical Chemistry C, 2015, 119, 16358-16365.	3.1	161
6	Thermal conductivities of single- and multi-layer phosphorene: a molecular dynamics study. Nanoscale, 2016, 8, 483-491.	5.6	159
7	Controlling of residual stress in additive manufacturing of Ti6Al4V by finite element modeling. Additive Manufacturing, 2016, 12, 231-239.	3.0	141
8	Effects of grain size, temperature and strain rate on the mechanical properties of polycrystalline graphene â€“ A molecular dynamics study. Carbon, 2015, 85, 135-146.	10.3	136
9	Nanometric cutting of copper: A molecular dynamics study. Computational Materials Science, 2006, 37, 434-441.	3.0	125
10	Large scale molecular dynamics study of nanometric machining of copper. Computational Materials Science, 2007, 41, 177-185.	3.0	120
11	Tuning the thermal conductivity of silicene with tensile strain and isotopic doping: A molecular dynamics study. Journal of Applied Physics, 2013, 114, .	2.5	118
12	Mechanical properties of methyl functionalized graphene: a molecular dynamics study. Nanotechnology, 2010, 21, 115709.	2.6	116
13	Interfacial thermal conductance in graphene/MoS2 heterostructures. Carbon, 2016, 96, 888-896.	10.3	116
14	Some Aspects of Thermal Transport across the Interface between Graphene and Epoxy in Nanocomposites. ACS Applied Materials & Interfaces, 2016, 8, 8272-8279.	8.0	106
15	An experimental and simulation study on build thickness dependent microstructure for electron beam melted Tiâ€“6Alâ€“4V. Journal of Alloys and Compounds, 2015, 646, 303-309.	5.5	105
16	Thermal conductivity of defective graphene. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 3668-3672.	2.1	103
17	Mechanical properties and fracture behavior of single-layer phosphorene at finite temperatures. Journal Physics D: Applied Physics, 2015, 48, 395303.	2.8	103
18	Effects of temperature and strain rate on the mechanical properties of silicene. Journal of Applied Physics, 2014, 115, .	2.5	100

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19	A molecular dynamics investigation on thermal conductivity of graphynes. Computational Materials Science, 2012, 65, 406-410.	3.0	92
20	Study of Materials Deformation in Nanometric Cutting by Large-scale Molecular Dynamics Simulations. Nanoscale Research Letters, 2009, 4, 444-451.	5.7	88
21	Carbon isotope doping induced interfacial thermal resistance and thermal rectification in graphene. Applied Physics Letters, 2012, 100, .	3.3	80
22	Inverse Pseudo Hall-Petch Relation in Polycrystalline Graphene. Scientific Reports, 2014, 4, 5991.	3.3	79
23	Thermal conductivity of fluorinated graphene: A non-equilibrium molecular dynamics study. Chemical Physics Letters, 2012, 552, 97-101.	2.6	77
24	Metallic glass-based chiral nanolattice: Light weight, auxeticity, and superior mechanical properties. Materials Today, 2017, 20, 569-576.	14.2	72
25	On the notch sensitivity of CuZr metallic glasses. Applied Physics Letters, 2013, 103, .	3.3	68
26	Necking and notch strengthening in metallic glass with symmetric sharp-and-deep notches. Scientific Reports, 2015, 5, 10797.	3.3	68
27	Atomistic origin of size effects in fatigue behavior of metallic glasses. Journal of the Mechanics and Physics of Solids, 2017, 104, 84-95.	4.8	68
28	In-plane and cross-plane thermal conductivities of molybdenum disulfide. Nanotechnology, 2015, 26, 065703.	2.6	67
29	Large-scale molecular dynamics simulations of wear in diamond-like carbon at the nanoscale. Applied Physics Letters, 2013, 103, .	3.3	59
30	On the failure load and mechanism of polycrystalline graphene by nanoindentation. Scientific Reports, 2014, 4, 7437.	3.3	58
31	A modified Tersoff potential for pure and hydrogenated diamond-like carbon. Computational Materials Science, 2013, 67, 146-150.	3.0	55
32	Ab initio molecular dynamics study of the local atomic structures in monatomic metallic liquid and glass. Materials & Design, 2015, 77, 1-5.	5.1	54
33	Atomic vacancies significantly degrade the mechanical properties of phosphorene. Nanotechnology, 2016, 27, 315704.	2.6	54
34	Predictive model for porosity in powder-bed fusion additive manufacturing at high beam energy regime. Additive Manufacturing, 2018, 22, 817-822.	3.0	54
35	A finite element study of the temperature rise during equal channel angular pressing. Scripta Materialia, 2003, 49, 303-308.	5.2	51
36	Effect of aspect ratio on the mechanical properties of metallic glasses. Scripta Materialia, 2014, 93, 36-39.	5.2	47

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37	Temperature and strain-rate dependent fracture strength of graphynes. Journal Physics D: Applied Physics, 2014, 47, 425301.	2.8	46
38	Crystallization of amorphous alloy during isothermal annealing: a molecular dynamics study. Journal of Physics Condensed Matter, 2005, 17, 1493-1504.	1.8	45
39	Is the failure of large-area polycrystalline graphene notch sensitive or insensitive?. Carbon, 2014, 72, 200-206.	10.3	45
40	Microstructure and Properties of Al-6061 Alloy by Equal Channel Angular Extrusion for 16 Passes. Materials and Manufacturing Processes, 2007, 22, 819-824.	4.7	44
41	Thermal conductivity of a h-BCN monolayer. Physical Chemistry Chemical Physics, 2017, 19, 27326-27331.	2.8	44
42	Recent progress in the development of thermal interface materials: a review. Physical Chemistry Chemical Physics, 2021, 23, 753-776.	2.8	44
43	Hydrogenated Grain Boundaries Control the Strength and Ductility of Polycrystalline Graphene. Journal of Physical Chemistry C, 2014, 118, 13769-13774.	3.1	43
44	Interfacial Thermal Conductance and Thermal Rectification of Hexagonal BC_nN/Graphene In-Plane Heterojunctions. Journal of Physical Chemistry C, 2018, 122, 22783-22789.	3.1	42
45	Modeling the Microstructure Evolution During Additive Manufacturing of Ti6Al4V: A Comparison Between Electron Beam Melting and Selective Laser Melting. Jom, 2016, 68, 1370-1375.	1.9	40
46	Graphene membranes with nanoslits for seawater desalinationviaforward osmosis. Physical Chemistry Chemical Physics, 2017, 19, 30551-30561.	2.8	40
47	Effect of elastic anisotropy on the elastic fields and vertical alignment of quantum dots. Journal of Applied Physics, 2003, 93, 1487-1492.	2.5	39
48	Strong and superplastic nanoglass. Nanoscale, 2015, 7, 17404-17409.	5.6	39
49	Notch strengthening in nanoscale metallic glasses. Acta Materialia, 2019, 169, 147-154.	7.9	39
50	Thermal stability and thermal conductivity of phosphorene in phosphorene/graphene van der Waals heterostructures. Physical Chemistry Chemical Physics, 2017, 19, 17180-17186.	2.8	37
51	The mechanical properties of a nanoglass/metallic glass/nanoglass sandwich structure. Scripta Materialia, 2014, 83, 37-40.	5.2	36
52	A molecular dynamics simulation study on thermal conductivity of functionalized bilayer graphene sheet. Chemical Physics Letters, 2015, 622, 104-108.	2.6	36
53	Mechanical properties and failure behaviour of graphene/silicene/graphene heterostructures. Journal Physics D: Applied Physics, 2017, 50, 345302.	2.8	36
54	Molecular dynamics study on the nanoimprint of copper. Journal Physics D: Applied Physics, 2007, 40, 4928-4935.	2.8	34

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55	Thermal conductivity of penta-graphene: The role of chemical functionalization. Computational Materials Science, 2017, 137, 195-200.	3.0	34
56	A molecular dynamics study of the mechanical properties of h-BCN monolayer using a modified Tersoff interatomic potential. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 2821-2827.	2.1	34
57	Tuning the thermal conductivity of multi-layer graphene with interlayer bonding and tensile strain. Applied Physics A: Materials Science and Processing, 2015, 120, 1275-1281.	2.3	32
58	Friction between silicon and diamond at the nanoscale. Journal Physics D: Applied Physics, 2015, 48, 255303.	2.8	30
59	Decoupled electron and phonon transports in hexagonal boron nitride-silicene bilayer heterostructure. Journal of Applied Physics, 2016, 119, .	2.5	29
60	Elastic properties of injection molded short glass fiber reinforced thermoplastic composites. Composite Structures, 2020, 254, 112850.	5.8	29
61	Effects of grain size and temperature on mechanical and failure properties of ultrananocrystalline diamond. Diamond and Related Materials, 2011, 20, 1303-1309.	3.9	28
62	Thermal transport behavior of polycrystalline graphene: A molecular dynamics study. Journal of Applied Physics, 2014, 116, .	2.5	28
63	Modeling and control of remelting in high-energy beam additive manufacturing. Additive Manufacturing, 2015, 7, 57-63.	3.0	28
64	The mechanical and thermal properties of MoS₂â€“WSe₂ lateral heterostructures. Physical Chemistry Chemical Physics, 2019, 21, 15845-15853.	2.8	28
65	Ab initio study on the electronic origin of glass-forming ability in the binary Cuâ€“Zr and the ternary Cuâ€“Zrâ€“Al(Ag) metallic glasses. Journal of Alloys and Compounds, 2015, 619, 16-19.	5.5	26
66	Temperature and strain-rate dependent mechanical properties of single-layer borophene. Extreme Mechanics Letters, 2018, 19, 39-45.	4.1	26
67	Molecular dynamics study on DNA oligonucleotide translocation through carbon nanotubes. Journal of Chemical Physics, 2008, 129, 125101.	3.0	24
68	Remarkable enhancement in failure stress and strain of penta-graphene via chemical functionalization. Nano Research, 2017, 10, 3865-3874.	10.4	24
69	Failure in Two-Dimensional Materials: Defect Sensitivity and Failure Criteria. Journal of Applied Mechanics, Transactions ASME, 2020, 87, .	2.2	24
70	Superplastic nanocrystalline ceramics at room temperature and high strain rates. Scripta Materialia, 2013, 69, 525-528.	5.2	22
71	A molecular dynamics investigation on mechanical properties of hydrogenated graphynes. Journal of Applied Physics, 2013, 114, .	2.5	22
72	Molecular Dynamics Simulations on the Frictional Behavior of a Perfluoropolyether Film Sandwiched between Diamond-like-Carbon Coatings. Langmuir, 2014, 30, 1573-1579.	3.5	21

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73	Anisotropic Wetting Characteristics of Water Droplets on Phosphorene: Roles of Layer and Defect Engineering. Journal of Physical Chemistry C, 2018, 122, 4622-4627.	3.1	21
74	The rapid solidification of Ti3Al : a molecular dynamics study. Journal of Physics Condensed Matter, 2004, 16, 4203-4210.	1.8	20
75	Deformation Behavior Study of Multi-Pass ECAE Process for Fabrication of Ultrafine or Nanostructured Bulk Materials. Materials and Manufacturing Processes, 2006, 21, 507-512.	4.7	20
76	Molecular-dynamics studies of competitive replacement in peptideâ€“nanotube assembly for control of drug release. Nanotechnology, 2009, 20, 145101.	2.6	20
77	On the notch sensitivity of CuZr nanoglass. Journal of Applied Physics, 2014, 115, .	2.5	20
78	A systematic study of interatomic potentials for mechanical behaviours of Ti-Al alloys. Computational Materials Science, 2021, 188, 110239.	3.0	20
79	Thermal transport in graphene-based layered materials: An analytical model validated with extensive molecular dynamics simulations. Carbon, 2019, 155, 114-121.	10.3	19
80	Interfacial thermal conductance in multilayer graphene/phosphorene heterostructure. Journal Physics D: Applied Physics, 2016, 49, 465301.	2.8	18
81	Unusual thermal properties of graphene origami crease: A molecular dynamics study. Green Energy and Environment, 2022, 7, 86-94.	8.7	18
82	Translocation of DNA oligonucleotide through carbon nanotube channels under induced pressure difference. Physica A: Statistical Mechanics and Its Applications, 2008, 387, 3111-3120.	2.6	17
83	The nature of the atomic-level structure in the Cuâ€“Zr binary metallic glasses. Intermetallics, 2012, 26, 8-10.	3.9	17
84	Deformation and failure mechanisms of nanoscale cellular structures of metallic glasses. RSC Advances, 2016, 6, 100899-100907.	3.6	14
85	Large diffusion anisotropy and orientation sorting of phosphorene nanoflakes under a temperature gradient. Nanoscale, 2018, 10, 1660-1666.	5.6	14
86	Active Control of Microstructure in Powderâ€Bed Fusion Additive Manufacturing of Ti6Al4V. Advanced Engineering Materials, 2017, 19, 1700333.	3.5	13
87	Modulating the thermal conductivity of silicon nanowires via surface amorphization. Science China Technological Sciences, 2014, 57, 699-705.	4.0	11
88	Mechanical behaviour of kirigami graphene under shear loading. Computational Materials Science, 2020, 173, 109462.	3.0	11
89	Composition-dependent effects of oxygen on atomic structure and mechanical properties of metallic glasses. Physical Chemistry Chemical Physics, 2021, 23, 1335-1342.	2.8	10
90	Simultaneously enhancing the strength and toughness of short fiber reinforced thermoplastic composites by fiber cross-linking. Composites Science and Technology, 2022, 217, 109076.	7.8	10

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91	Defect-Engineered Thermal Transport in Wrinkled Graphene: A Comprehensive Molecular Dynamics Study. Journal of Physical Chemistry C, 2022, 126, 5759-5766.	3.1	10
92	Thermal conductivity of oxidized gamma-graphyne. RSC Advances, 2015, 5, 65221-65226.	3.6	9
93	Failure Mechanism of Phosphorene by Nanoindentation. Journal of Physical Chemistry C, 2017, 121, 4708-4713.	3.1	9
94	Exploring the structureâ€“property relationship of three-dimensional hexagonal boron nitride aerogels with gyroid surfaces. Nanoscale, 2020, 12, 10180-10188.	5.6	9
95	Effect of surface coupling agents on the mechanical behaviour of polypropylene/silica composites: a molecular dynamics study. Journal of Polymer Research, 2021, 28, 1.	2.4	9
96	Atomistic Molecular Dynamics Study of Structural and Thermomechanical Properties of Zdol Lubricants on Hydrogenated Diamond-Like Carbon. IEEE Transactions on Magnetics, 2013, 49, 5227-5235.	2.1	8
97	Thermal damage and ablation behavior of graphene induced by ultrafast laser irradiation. Journal of Thermal Stresses, 2018, 41, 1153-1168.	2.0	8
98	Coupled Thermo-Mechanical Analysis of Severe Plastic Deformation for Producing Bulk Nanostructured Materials. Advanced Engineering Materials, 2004, 6, 933-936.	3.5	7
99	Effect of sp3-hybridized defects on the oscillatory behavior of carbon nanotube oscillators. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 2400-2404.	2.1	7
100	Intrinsic and extrinsic effects on the fracture toughness of ductile metallic glasses. Mechanics of Materials, 2021, 162, 104066.	3.2	7
101	Strength and buckling behavior of defective phosphorene nanotubes under axial compression. Journal of Materials Science, 2018, 53, 8355-8363.	3.7	6
102	Mechanical properties and fracture behaviour of defective phosphorene nanotubes under uniaxial tension. Journal Physics D: Applied Physics, 2017, 50, 485303.	2.8	6
103	Surface morphology and strain coupling effects on phonon transport in silicon nanowires. Materials Today: Proceedings, 2016, 3, 2759-2765.	1.8	5
104	Temperature and defect effects on the mechanical properties of pentadiamond. Diamond and Related Materials, 2021, 118, 108523.	3.9	5
105	Elastic fields in quantum dots arrays: A three-dimensional finite element study. Engineering Analysis With Boundary Elements, 2008, 32, 309-317.	3.7	4
106	Simulations of micro and nanoindentations. Journal of Mechanics of Materials and Structures, 2008, 3, 1847-1856.	0.6	4
107	Atomistic-scale analysis of the deformation and failure of polypropylene composites reinforced by functionalized silica nanoparticles. Scientific Reports, 2021, 11, 23108.	3.3	4
108	Thermo-Mechanical Modeling and Analysis of Equal Channel Angular Pressing. Journal of Metastable and Nanocrystalline Materials, 2005, 23, 263-266.	0.1	2

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109	STUDY ON NANOMETRIC CUTTING MECHANISM AND BURR FORMATION USING MOLECULAR DYNAMICS SIMULATION. International Journal of Nanoscience, 2006, 05, 547-551.	0.7	2
110	Modeling and Analysis of the Geometryâ€Dependent Mechanical and Thermal Properties of Coiled Carbon Nanotubes. Physica Status Solidi - Rapid Research Letters, 0, , 2100360.	2.4	2
111	MOLECULAR DYNAMICS SIMULATION OF NANOMETRIC CUTTING PROCESS. International Journal of Nanoscience, 2006, 05, 633-638.	0.7	1
112	Modelling of Defects and Failure in 2D Materials: Graphene and Beyond. , 2018, , 1-41.		1
113	Modelling of Defects and Failure in 2D Materials: Graphene and Beyond. , 2020, , 1869-1909.		1
114	Study of Direct Nanoimprinting Processes by Molecular Dynamics Simulations. Journal of Computational and Theoretical Nanoscience, 2010, 7, 2144-2150.	0.4	0
115	MECHANICAL PROPERTIES AND FRACTURE BEHAVIOR OF GRAPHENE AND OTHER 2D MATERIALS. , 2015, , 75-76.		0
116	Notch Strengthening in Nanoscale Metallic Glasses. SSRN Electronic Journal, 2018, , .	0.4	0
117	Temperature and Defect Effects on the Mechanical Properties of Pentadiamond. SSRN Electronic Journal, 0, , .	0.4	0
118	THREE-DIMENSIONAL FINITE ELEMENT STUDY OF THE ELASTIC FIELDS IN QUANTUM DOT STRUCTURES. , 2002, , .		0
119	Energy Dissipation Analysis of Defected Carbon Nanotube Oscillators. , 2012, , .		0