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	Unusual thermal properties of graphene origami crease: A molecular dynamics study. Green Energy and Environment, 2022, 7, 86-94.	8.7	18
2	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
3	Defect-Engineered Thermal Transport in Wrinkled Graphene: A Comprehensive Molecular Dynamics Study. Journal of Physical Chemistry C, 2022, 126, 5759-5766.	3.1	10
4	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
5	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
6	A systematic study of interatomic potentials for mechanical behaviours of Ti-Al alloys. Computational Materials Science, 2021, 188, 110239.	3.0	20
7	Temperature and defect effects on the mechanical properties of pentadiamond. Diamond and Related Materials, 2021, 118, 108523.	3.9	5
8	Intrinsic and extrinsic effects on the fracture toughness of ductile metallic glasses. Mechanics of Materials, 2021, 162, 104066.	3.2	7
9	Recent progress in the development of thermal interface materials: a review. Physical Chemistry Chemical Physics, 2021, 23, 753-776.	2.8	44
10	Atomistic-scale analysis of the deformation and failure of polypropylene composites reinforced by functionalized silica nanoparticles. Scientific Reports, 2021, 11, 23108.	3.3	4
11	Mechanical behaviour of kirigami graphene under shear loading. Computational Materials Science, 2020, 173, 109462.	3.0	11
12	Elastic properties of injection molded short glass fiber reinforced thermoplastic composites. Composite Structures, 2020, 254, 112850.	5.8	29
13	Exploring the structureâ€“property relationship of three-dimensional hexagonal boron nitride aerogels with gyroid surfaces. Nanoscale, 2020, 12, 10180-10188.	5.6	9
14	Modelling of Defects and Failure in 2D Materials: Graphene and Beyond. , 2020, , 1869-1909.		1
15	Failure in Two-Dimensional Materials: Defect Sensitivity and Failure Criteria. Journal of Applied Mechanics, Transactions ASME, 2020, 87, .	2.2	24
16	Thermal transport in graphene-based layered materials: An analytical model validated with extensive molecular dynamics simulations. Carbon, 2019, 155, 114-121.	10.3	19
17	The mechanical and thermal properties of MoS₂â€“WSe₂ lateral heterostructures. Physical Chemistry Chemical Physics, 2019, 21, 15845-15853.	2.8	28
18	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

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19	Notch strengthening in nanoscale metallic glasses. Acta Materialia, 2019, 169, 147-154.	7.9	39
20	Strength and buckling behavior of defective phosphorene nanotubes under axial compression. Journal of Materials Science, 2018, 53, 8355-8363.	3.7	6
21	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
22	Temperature and strain-rate dependent mechanical properties of single-layer borophene. Extreme Mechanics Letters, 2018, 19, 39-45.	4.1	26
23	Large diffusion anisotropy and orientation sorting of phosphorene nanoflakes under a temperature gradient. Nanoscale, 2018, 10, 1660-1666.	5.6	14
24	Notch Strengthening in Nanoscale Metallic Glasses. SSRN Electronic Journal, 2018, , .	0.4	0
25	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
26	Predictive model for porosity in powder-bed fusion additive manufacturing at high beam energy regime. Additive Manufacturing, 2018, 22, 817-822.	3.0	54
27	Thermal damage and ablation behavior of graphene induced by ultrafast laser irradiation. Journal of Thermal Stresses, 2018, 41, 1153-1168.	2.0	8
28	Modelling of Defects and Failure in 2D Materials: Graphene and Beyond. , 2018, , 1-41.		1
29	Failure Mechanism of Phosphorene by Nanoindentation. Journal of Physical Chemistry C, 2017, 121, 4708-4713.	3.1	9
30	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
31	Remarkable enhancement in failure stress and strain of penta-graphene via chemical functionalization. Nano Research, 2017, 10, 3865-3874.	10.4	24
32	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
33	Graphene membranes with nanoslits for seawater desalinationviaforward osmosis. Physical Chemistry Chemical Physics, 2017, 19, 30551-30561.	2.8	40
34	Thermal conductivity of a h-BCN monolayer. Physical Chemistry Chemical Physics, 2017, 19, 27326-27331.	2.8	44
35	Active Control of Microstructure in Powderâ€Bed Fusion Additive Manufacturing of Ti6Al4V. Advanced Engineering Materials, 2017, 19, 1700333.	3.5	13
36	Metallic glass-based chiral nanolattice: Light weight, auxeticity, and superior mechanical properties. Materials Today, 2017, 20, 569-576.	14.2	72

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37	Mechanical properties and failure behaviour of graphene/silicene/graphene heterostructures. Journal Physics D: Applied Physics, 2017, 50, 345302.	2.8	36
38	Thermal conductivity of penta-graphene: The role of chemical functionalization. Computational Materials Science, 2017, 137, 195-200.	3.0	34
39	Mechanical properties and fracture behaviour of defective phosphorene nanotubes under uniaxial tension. Journal Physics D: Applied Physics, 2017, 50, 485303.	2.8	6
40	Atomic vacancies significantly degrade the mechanical properties of phosphorene. Nanotechnology, 2016, 27, 315704.	2.6	54
41	Decoupled electron and phonon transports in hexagonal boron nitride-silicene bilayer heterostructure. Journal of Applied Physics, 2016, 119, .	2.5	29
42	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
43	Controlling of residual stress in additive manufacturing of Ti6Al4V by finite element modeling. Additive Manufacturing, 2016, 12, 231-239.	3.0	141
44	Surface morphology and strain coupling effects on phonon transport in silicon nanowires. Materials Today: Proceedings, 2016, 3, 2759-2765.	1.8	5
45	Deformation and failure mechanisms of nanoscale cellular structures of metallic glasses. RSC Advances, 2016, 6, 100899-100907.	3.6	14
46	Interfacial thermal conductance in multilayer graphene/phosphorene heterostructure. Journal Physics D: Applied Physics, 2016, 49, 465301.	2.8	18
47	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
48	Thermal conductivities of single- and multi-layer phosphorene: a molecular dynamics study. Nanoscale, 2016, 8, 483-491.	5.6	159
49	Interfacial thermal conductance in graphene/MoS2 heterostructures. Carbon, 2016, 96, 888-896.	10.3	116
50	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
51	MECHANICAL PROPERTIES AND FRACTURE BEHAVIOR OF GRAPHENE AND OTHER 2D MATERIALS. , 2015, , 75-76.		0
52	Friction between silicon and diamond at the nanoscale. Journal Physics D: Applied Physics, 2015, 48, 255303.	2.8	30
53	Mechanical properties and fracture behavior of single-layer phosphorene at finite temperatures. Journal Physics D: Applied Physics, 2015, 48, 395303.	2.8	103
54	A molecular dynamics simulation study on thermal conductivity of functionalized bilayer graphene sheet. Chemical Physics Letters, 2015, 622, 104-108.	2.6	36

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55	In-plane and cross-plane thermal conductivities of molybdenum disulfide. Nanotechnology, 2015, 26, 065703.	2.6	67
56	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
57	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
58	Thermal conductivity of oxidized gamma-graphyne. RSC Advances, 2015, 5, 65221-65226.	3.6	9
59	Necking and notch strengthening in metallic glass with symmetric sharp-and-deep notches. Scientific Reports, 2015, 5, 10797.	3.3	68
60	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
61	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
62	Strong and superplastic nanoglass. Nanoscale, 2015, 7, 17404-17409.	5.6	39
63	Modeling and control of remelting in high-energy beam additive manufacturing. Additive Manufacturing, 2015, 7, 57-63.	3.0	28
64	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
65	Effect of aspect ratio on the mechanical properties of metallic glasses. Scripta Materialia, 2014, 93, 36-39.	5.2	47
66	Thermal transport behavior of polycrystalline graphene: A molecular dynamics study. Journal of Applied Physics, 2014, 116, .	2.5	28
67	The mechanical properties of a nanoglass/metallic glass/nanoglass sandwich structure. Scripta Materialia, 2014, 83, 37-40.	5.2	36
68	Modulating the thermal conductivity of silicon nanowires via surface amorphization. Science China Technological Sciences, 2014, 57, 699-705.	4.0	11
69	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
70	Temperature and strain-rate dependent fracture strength of graphynes. Journal Physics D: Applied Physics, 2014, 47, 425301.	2.8	46
71	Effects of temperature and strain rate on the mechanical properties of silicene. Journal of Applied Physics, 2014, 115, .	2.5	100
72	Is the failure of large-area polycrystalline graphene notch sensitive or insensitive?. Carbon, 2014, 72, 200-206.	10.3	45

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73	Hydrogenated Grain Boundaries Control the Strength and Ductility of Polycrystalline Graphene. Journal of Physical Chemistry C, 2014, 118, 13769-13774.	3.1	43
74	On the notch sensitivity of CuZr nanoglass. Journal of Applied Physics, 2014, 115, .	2.5	20
75	Inverse Pseudo Hall-Petch Relation in Polycrystalline Graphene. Scientific Reports, 2014, 4, 5991.	3.3	79
76	On the failure load and mechanism of polycrystalline graphene by nanoindentation. Scientific Reports, 2014, 4, 7437.	3.3	58
77	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
78	On the notch sensitivity of CuZr metallic glasses. Applied Physics Letters, 2013, 103, .	3.3	68
79	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
80	Phonon thermal conductivity of monolayer MoS₂ sheet and nanoribbons. Applied Physics Letters, 2013, 103, 133113.	3.3	167
81	Superplastic nanocrystalline ceramics at room temperature and high strain rates. Scripta Materialia, 2013, 69, 525-528.	5.2	22
82	A modified Tersoff potential for pure and hydrogenated diamond-like carbon. Computational Materials Science, 2013, 67, 146-150.	3.0	55
83	A molecular dynamics investigation on mechanical properties of hydrogenated graphynes. Journal of Applied Physics, 2013, 114, .	2.5	22
84	Large-scale molecular dynamics simulations of wear in diamond-like carbon at the nanoscale. Applied Physics Letters, 2013, 103, .	3.3	59
85	Thermal conductivity of fluorinated graphene: A non-equilibrium molecular dynamics study. Chemical Physics Letters, 2012, 552, 97-101.	2.6	77
86	The nature of the atomic-level structure in the Cuâ€“Zr binary metallic glasses. Intermetallics, 2012, 26, 8-10.	3.9	17
87	Mechanical properties of graphynes under tension: A molecular dynamics study. Applied Physics Letters, 2012, 101, 081909.	3.3	217
88	A molecular dynamics investigation on thermal conductivity of graphynes. Computational Materials Science, 2012, 65, 406-410.	3.0	92
89	Thermal conductivity of defective graphene. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 3668-3672.	2.1	103
90	Carbon isotope doping induced interfacial thermal resistance and thermal rectification in graphene. Applied Physics Letters, 2012, 100, .	3.3	80

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91	Energy Dissipation Analysis of Defected Carbon Nanotube Oscillators. , 2012, , .		0
92	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
93	A theoretical analysis of the thermal conductivity of hydrogenated graphene. Carbon, 2011, 49, 4752-4759.	10.3	176
94	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
95	Study of Direct Nanoimprinting Processes by Molecular Dynamics Simulations. Journal of Computational and Theoretical Nanoscience, 2010, 7, 2144-2150.	0.4	0
96	A molecular dynamics study of the mechanical properties of hydrogen functionalized graphene. Carbon, 2010, 48, 898-904.	10.3	442
97	Mechanical properties of methyl functionalized graphene: a molecular dynamics study. Nanotechnology, 2010, 21, 115709.	2.6	116
98	Study of Materials Deformation in Nanometric Cutting by Large-scale Molecular Dynamics Simulations. Nanoscale Research Letters, 2009, 4, 444-451.	5.7	88
99	Molecular-dynamics studies of competitive replacement in peptideâ€“nanotube assembly for control of drug release. Nanotechnology, 2009, 20, 145101.	2.6	20
100	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
101	Elastic fields in quantum dots arrays: A three-dimensional finite element study. Engineering Analysis With Boundary Elements, 2008, 32, 309-317.	3.7	4
102	Molecular dynamics study on DNA oligonucleotide translocation through carbon nanotubes. Journal of Chemical Physics, 2008, 129, 125101.	3.0	24
103	Simulations of micro and nanoindentations. Journal of Mechanics of Materials and Structures, 2008, 3, 1847-1856.	0.6	4
104	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
105	Molecular dynamics study on the nanoimprint of copper. Journal Physics D: Applied Physics, 2007, 40, 4928-4935.	2.8	34
106	Large scale molecular dynamics study of nanometric machining of copper. Computational Materials Science, 2007, 41, 177-185.	3.0	120
107	Nanometric cutting of copper: A molecular dynamics study. Computational Materials Science, 2006, 37, 434-441.	3.0	125
108	MOLECULAR DYNAMICS SIMULATION OF NANOMETRIC CUTTING PROCESS. International Journal of Nanoscience, 2006, 05, 633-638.	0.7	1

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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	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
111	Thermo-Mechanical Modeling and Analysis of Equal Channel Angular Pressing. Journal of Metastable and Nanocrystalline Materials, 2005, 23, 263-266.	0.1	2
112	Crystallization of amorphous alloy during isothermal annealing: a molecular dynamics study. Journal of Physics Condensed Matter, 2005, 17, 1493-1504.	1.8	45
113	Coupled Thermo-Mechanical Analysis of Severe Plastic Deformation for Producing Bulk Nanostructured Materials. Advanced Engineering Materials, 2004, 6, 933-936.	3.5	7
114	The rapid solidification of Ti3Al : a molecular dynamics study. Journal of Physics Condensed Matter, 2004, 16, 4203-4210.	1.8	20
115	A finite element study of the temperature rise during equal channel angular pressing. Scripta Materialia, 2003, 49, 303-308.	5.2	51
116	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
117	THREE-DIMENSIONAL FINITE ELEMENT STUDY OF THE ELASTIC FIELDS IN QUANTUM DOT STRUCTURES. , 2002, , .		0
118	Temperature and Defect Effects on the Mechanical Properties of Pentadiamond. SSRN Electronic Journal, 0, , .	0.4	0
119	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