

# Qing-Xia Pei

## List of Publications by Citations

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114  
papers

4,389  
citations

38  
h-index

62  
g-index

119  
ext. papers

4,920  
ext. citations

4.2  
avg, IF

5.91  
L-index

#	Paper	IF	Citations
114	A molecular dynamics study of the mechanical properties of hydrogen functionalized graphene. <i>Carbon</i> , <b>2010</b> , 48, 898-904	10.4	390
113	Mechanical properties of graphynes under tension: A molecular dynamics study. <i>Applied Physics Letters</i> , <b>2012</b> , 101, 081909	3.4	184
112	A theoretical analysis of the thermal conductivity of hydrogenated graphene. <i>Carbon</i> , <b>2011</b> , 49, 4752-4758	10.4	152
111	Phonon thermal conductivity of monolayer MoS2 sheet and nanoribbons. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 133113	3.4	145
110	Thermal conductivities of single- and multi-layer phosphorene: a molecular dynamics study. <i>Nanoscale</i> , <b>2016</b> , 8, 483-91	7.7	129
109	Manipulating the Thermal Conductivity of Monolayer MoS2 via Lattice Defect and Strain Engineering. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 16358-16365	3.8	112
108	Controlling of residual stress in additive manufacturing of Ti6Al4V by finite element modeling. <i>Additive Manufacturing</i> , <b>2016</b> , 12, 231-239	6.1	106
107	Tuning the thermal conductivity of silicene with tensile strain and isotopic doping: A molecular dynamics study. <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 033526	2.5	102
106	Large scale molecular dynamics study of nanometric machining of copper. <i>Computational Materials Science</i> , <b>2007</b> , 41, 177-185	3.2	101
105	Nanometric cutting of copper: A molecular dynamics study. <i>Computational Materials Science</i> , <b>2006</b> , 37, 434-441	3.2	101
104	Effects of grain size, temperature and strain rate on the mechanical properties of polycrystalline graphene [A molecular dynamics study. <i>Carbon</i> , <b>2015</b> , 85, 135-146	10.4	96
103	Effects of temperature and strain rate on the mechanical properties of silicene. <i>Journal of Applied Physics</i> , <b>2014</b> , 115, 023519	2.5	93
102	Mechanical properties of methyl functionalized graphene: a molecular dynamics study. <i>Nanotechnology</i> , <b>2010</b> , 21, 115709	3.4	92
101	Mechanical properties and fracture behavior of single-layer phosphorene at finite temperatures. <i>Journal Physics D: Applied Physics</i> , <b>2015</b> , 48, 395303	3	86
100	Study of Materials Deformation in Nanometric Cutting by Large-scale Molecular Dynamics Simulations. <i>Nanoscale Research Letters</i> , <b>2009</b> , 4, 444-451	5	82
99	An experimental and simulation study on build thickness dependent microstructure for electron beam melted Ti6Al4V. <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 646, 303-309	5.7	81
98	A molecular dynamics investigation on thermal conductivity of graphynes. <i>Computational Materials Science</i> , <b>2012</b> , 65, 406-410	3.2	80

97	Thermal conductivity of defective graphene. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2012</b> , 376, 3668-3672	2.3	78
96	Interfacial thermal conductance in graphene/MoS2 heterostructures. <i>Carbon</i> , <b>2016</b> , 96, 888-896	10.4	77
95	Carbon isotope doping induced interfacial thermal resistance and thermal rectification in graphene. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 101901	3.4	73
94	Some Aspects of Thermal Transport across the Interface between Graphene and Epoxy in Nanocomposites. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 8272-9	9.5	71
93	Inverse pseudo Hall-Petch relation in polycrystalline graphene. <i>Scientific Reports</i> , <b>2014</b> , 4, 5991	4.9	67
92	Thermal conductivity of fluorinated graphene: A non-equilibrium molecular dynamics study. <i>Chemical Physics Letters</i> , <b>2012</b> , 552, 97-101	2.5	61
91	On the notch sensitivity of CuZr metallic glasses. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 081903	3.4	60
90	Necking and notch strengthening in metallic glass with symmetric sharp-and-deep notches. <i>Scientific Reports</i> , <b>2015</b> , 5, 10797	4.9	56
89	Metallic glass-based chiral nanolattice: Light weight, auxeticity, and superior mechanical properties. <i>Materials Today</i> , <b>2017</b> , 20, 569-576	21.8	56
88	Large-scale molecular dynamics simulations of wear in diamond-like carbon at the nanoscale. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 073118	3.4	55
87	In-plane and cross-plane thermal conductivities of molybdenum disulfide. <i>Nanotechnology</i> , <b>2015</b> , 26, 065703	3.4	53
86	Atomistic origin of size effects in fatigue behavior of metallic glasses. <i>Journal of the Mechanics and Physics of Solids</i> , <b>2017</b> , 104, 84-95	5	52
85	On the failure load and mechanism of polycrystalline graphene by nanoindentation. <i>Scientific Reports</i> , <b>2014</b> , 4, 7437	4.9	48
84	Ab initio molecular dynamics study of the local atomic structures in monatomic metallic liquid and glass. <i>Materials &amp; Design</i> , <b>2015</b> , 77, 1-5		47
83	A finite element study of the temperature rise during equal channel angular pressing. <i>Scripta Materialia</i> , <b>2003</b> , 49, 303-308	5.6	47
82	Atomic vacancies significantly degrade the mechanical properties of phosphorene. <i>Nanotechnology</i> , <b>2016</b> , 27, 315704	3.4	44
81	Predictive model for porosity in powder-bed fusion additive manufacturing at high beam energy regime. <i>Additive Manufacturing</i> , <b>2018</b> , 22, 817-822	6.1	41
80	Crystallization of amorphous alloy during isothermal annealing: a molecular dynamics study. <i>Journal of Physics Condensed Matter</i> , <b>2005</b> , 17, 1493-1504	1.8	40

79	Hydrogenated Grain Boundaries Control the Strength and Ductility of Polycrystalline Graphene. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 13769-13774	3.8	39
78	Effect of aspect ratio on the mechanical properties of metallic glasses. <i>Scripta Materialia</i> , <b>2014</b> , 93, 36-39	3.6	38
77	Microstructure and Properties of Al-6061 Alloy by Equal Channel Angular Extrusion for 16 Passes. <i>Materials and Manufacturing Processes</i> , <b>2007</b> , 22, 819-824	4.1	38
76	Temperature and strain-rate dependent fracture strength of graphynes. <i>Journal Physics D: Applied Physics</i> , <b>2014</b> , 47, 425301	3	37
75	A modified Tersoff potential for pure and hydrogenated diamond-like carbon. <i>Computational Materials Science</i> , <b>2013</b> , 67, 146-150	3.2	37
74	Is the failure of large-area polycrystalline graphene notch sensitive or insensitive?. <i>Carbon</i> , <b>2014</b> , 72, 200-206	10.4	36
73	Effect of elastic anisotropy on the elastic fields and vertical alignment of quantum dots. <i>Journal of Applied Physics</i> , <b>2003</b> , 93, 1487-1492	2.5	36
72	Modeling the Microstructure Evolution During Additive Manufacturing of Ti6Al4V: A Comparison Between Electron Beam Melting and Selective Laser Melting. <i>Jom</i> , <b>2016</b> , 68, 1370-1375	2.1	34
71	The mechanical properties of a nanoglass/metallic glass/nanoglass sandwich structure. <i>Scripta Materialia</i> , <b>2014</b> , 83, 37-40	5.6	32
70	Strong and superplastic nanoglass. <i>Nanoscale</i> , <b>2015</b> , 7, 17404-9	7.7	31
69	Molecular dynamics study on the nanoimprint of copper. <i>Journal Physics D: Applied Physics</i> , <b>2007</b> , 40, 4928-4935	3	31
68	Graphene membranes with nanoslits for seawater desalination via forward osmosis. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 30551-30561	3.6	30
67	Thermal conductivity of a h-BCN monolayer. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 27326-27331	3.6	27
66	Mechanical properties and failure behaviour of graphene/silicene/graphene heterostructures. <i>Journal Physics D: Applied Physics</i> , <b>2017</b> , 50, 345302	3	27
65	A molecular dynamics simulation study on thermal conductivity of functionalized bilayer graphene sheet. <i>Chemical Physics Letters</i> , <b>2015</b> , 622, 104-108	2.5	27
64	Thermal stability and thermal conductivity of phosphorene in phosphorene/graphene van der Waals heterostructures. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 17180-17186	3.6	26
63	Notch strengthening in nanoscale metallic glasses. <i>Acta Materialia</i> , <b>2019</b> , 169, 147-154	8.4	26
62	Effects of grain size and temperature on mechanical and failure properties of ultrananocrystalline diamond. <i>Diamond and Related Materials</i> , <b>2011</b> , 20, 1303-1309	3.5	25

61	Decoupled electron and phonon transports in hexagonal boron nitride-silicene bilayer heterostructure. <i>Journal of Applied Physics</i> , <b>2016</b> , 119, 065102	2.5	25
60	Interfacial Thermal Conductance and Thermal Rectification of Hexagonal BC <sub>n</sub> N/Graphene In-Plane Heterojunctions. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 22783-22789	3.8	24
59	Ab initio study on the electronic origin of glass-forming ability in the binary Cu <sub>2</sub> Zr and the ternary Cu <sub>2</sub> ZrAl(Ag) metallic glasses. <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 619, 16-19	5.7	23
58	Thermal conductivity of penta-graphene: The role of chemical functionalization. <i>Computational Materials Science</i> , <b>2017</b> , 137, 195-200	3.2	23
57	Thermal transport behavior of polycrystalline graphene: A molecular dynamics study. <i>Journal of Applied Physics</i> , <b>2014</b> , 116, 204303	2.5	23
56	Molecular dynamics study on DNA oligonucleotide translocation through carbon nanotubes. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 125101	3.9	23
55	Tuning the thermal conductivity of multi-layer graphene with interlayer bonding and tensile strain. <i>Applied Physics A: Materials Science and Processing</i> , <b>2015</b> , 120, 1275-1281	2.6	22
54	Modeling and control of remelting in high-energy beam additive manufacturing. <i>Additive Manufacturing</i> , <b>2015</b> , 7, 57-63	6.1	20
53	Temperature and strain-rate dependent mechanical properties of single-layer borophene. <i>Extreme Mechanics Letters</i> , <b>2018</b> , 19, 39-45	3.9	20
52	Friction between silicon and diamond at the nanoscale. <i>Journal Physics D: Applied Physics</i> , <b>2015</b> , 48, 255303	3.9	20
51	Deformation Behavior Study of Multi-Pass ECAE Process for Fabrication of Ultrafine or Nanostructured Bulk Materials. <i>Materials and Manufacturing Processes</i> , <b>2006</b> , 21, 507-512	4.1	19
50	The rapid solidification of Ti <sub>3</sub> Al : a molecular dynamics study. <i>Journal of Physics Condensed Matter</i> , <b>2004</b> , 16, 4203-4210	1.8	19
49	Recent progress in the development of thermal interface materials: a review. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 753-776	3.6	19
48	On the notch sensitivity of CuZr nanoglass. <i>Journal of Applied Physics</i> , <b>2014</b> , 115, 163507	2.5	18
47	A molecular dynamics investigation on mechanical properties of hydrogenated graphynes. <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 073504	2.5	18
46	Molecular-dynamics studies of competitive replacement in peptide-nanotube assembly for control of drug release. <i>Nanotechnology</i> , <b>2009</b> , 20, 145101	3.4	18
45	Remarkable enhancement in failure stress and strain of penta-graphene via chemical functionalization. <i>Nano Research</i> , <b>2017</b> , 10, 3865-3874	10	17
44	A molecular dynamics study of the mechanical properties of h-BCN monolayer using a modified Tersoff interatomic potential. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2019</b> , 383, 2821-2827	2.3	17

43	Anisotropic Wetting Characteristics of Water Droplets on Phosphorene: Roles of Layer and Defect Engineering. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 4622-4627	3.8	17
42	Translocation of DNA oligonucleotide through carbon nanotube channels under induced pressure difference. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2008</b> , 387, 3111-3120	3.3	17
41	Superplastic nanocrystalline ceramics at room temperature and high strain rates. <i>Scripta Materialia</i> , <b>2013</b> , 69, 525-528	5.6	16
40	The mechanical and thermal properties of MoS-WSe lateral heterostructures. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 15845-15853	3.6	15
39	The nature of the atomic-level structure in the CuZr binary metallic glasses. <i>Intermetallics</i> , <b>2012</b> , 26, 8-10	3.5	15
38	Molecular dynamics simulations on the frictional behavior of a perfluoropolyether film sandwiched between diamond-like-carbon coatings. <i>Langmuir</i> , <b>2014</b> , 30, 1573-9	4	14
37	Deformation and failure mechanisms of nanoscale cellular structures of metallic glasses. <i>RSC Advances</i> , <b>2016</b> , 6, 100899-100907	3.7	13
36	Large diffusion anisotropy and orientation sorting of phosphorene nanoflakes under a temperature gradient. <i>Nanoscale</i> , <b>2018</b> , 10, 1660-1666	7.7	12
35	Interfacial thermal conductance in multilayer graphene/phosphorene heterostructure. <i>Journal Physics D: Applied Physics</i> , <b>2016</b> , 49, 465301	3	12
34	Active Control of Microstructure in Powder-Bed Fusion Additive Manufacturing of Ti6Al4V. <i>Advanced Engineering Materials</i> , <b>2017</b> , 19, 1700333	3.5	12
33	A systematic study of interatomic potentials for mechanical behaviours of Ti-Al alloys. <i>Computational Materials Science</i> , <b>2021</b> , 188, 110239	3.2	11
32	Modulating the thermal conductivity of silicon nanowires via surface amorphization. <i>Science China Technological Sciences</i> , <b>2014</b> , 57, 699-705	3.5	10
31	Elastic properties of injection molded short glass fiber reinforced thermoplastic composites. <i>Composite Structures</i> , <b>2020</b> , 254, 112850	5.3	10
30	Thermal transport in graphene-based layered materials: An analytical model validated with extensive molecular dynamics simulations. <i>Carbon</i> , <b>2019</b> , 155, 114-121	10.4	8
29	Atomistic Molecular Dynamics Study of Structural and Thermomechanical Properties of Zdol Lubricants on Hydrogenated Diamond-Like Carbon. <i>IEEE Transactions on Magnetics</i> , <b>2013</b> , 49, 5227-5235 <sup>2</sup>		8
28	Failure in Two-Dimensional Materials: Defect Sensitivity and Failure Criteria. <i>Journal of Applied Mechanics, Transactions ASME</i> , <b>2020</b> , 87,	2.7	8
27	Thermal conductivity of oxidized gamma-graphyne. <i>RSC Advances</i> , <b>2015</b> , 5, 65221-65226	3.7	7
26	Coupled Thermo-Mechanical Analysis of Severe Plastic Deformation for Producing Bulk Nanostructured Materials. <i>Advanced Engineering Materials</i> , <b>2004</b> , 6, 933-936	3.5	7

25	Composition-dependent effects of oxygen on atomic structure and mechanical properties of metallic glasses. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 1335-1342	3.6	7
24	Strength and buckling behavior of defective phosphorene nanotubes under axial compression. <i>Journal of Materials Science</i> , <b>2018</b> , 53, 8355-8363	4.3	6
23	Failure Mechanism of Phosphorene by Nanoindentation. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 4708-4713	3.4	5
22	Thermal damage and ablation behavior of graphene induced by ultrafast laser irradiation. <i>Journal of Thermal Stresses</i> , <b>2018</b> , 41, 1153-1168	2.2	5
21	Effect of sp <sup>3</sup> -hybridized defects on the oscillatory behavior of carbon nanotube oscillators. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2011</b> , 375, 2400-2404	2.3	5
20	Unusual thermal properties of graphene origami crease: A molecular dynamics study. <i>Green Energy and Environment</i> , <b>2020</b> ,	5.7	5
19	Simulations of micro and nanoindentations. <i>Journal of Mechanics of Materials and Structures</i> , <b>2008</b> , 3, 1847-1856	1.2	4
18	Elastic fields in quantum dots arrays: A three-dimensional finite element study. <i>Engineering Analysis With Boundary Elements</i> , <b>2008</b> , 32, 309-317	2.6	4
17	Simultaneously enhancing the strength and toughness of short fiber reinforced thermoplastic composites by fiber cross-linking. <i>Composites Science and Technology</i> , <b>2022</b> , 217, 109076	8.6	4
16	Mechanical properties and fracture behaviour of defective phosphorene nanotubes under uniaxial tension. <i>Journal Physics D: Applied Physics</i> , <b>2017</b> , 50, 485303	3	4
15	Mechanical behaviour of kirigami graphene under shear loading. <i>Computational Materials Science</i> , <b>2020</b> , 173, 109462	3.2	4
14	Surface morphology and strain coupling effects on phonon transport in silicon nanowires. <i>Materials Today: Proceedings</i> , <b>2016</b> , 3, 2759-2765	1.4	4
13	Temperature and defect effects on the mechanical properties of pentadiamond. <i>Diamond and Related Materials</i> , <b>2021</b> , 118, 108523	3.5	4
12	Exploring the structure-property relationship of three-dimensional hexagonal boron nitride aerogels with gyroid surfaces. <i>Nanoscale</i> , <b>2020</b> , 12, 10180-10188	7.7	3
11	Effect of surface coupling agents on the mechanical behaviour of polypropylene/silica composites: a molecular dynamics study. <i>Journal of Polymer Research</i> , <b>2021</b> , 28, 1	2.7	2
10	Intrinsic and extrinsic effects on the fracture toughness of ductile metallic glasses. <i>Mechanics of Materials</i> , <b>2021</b> , 162, 104066	3.3	2
9	Modelling of Defects and Failure in 2D Materials: Graphene and Beyond <b>2018</b> , 1-41		1
8	MOLECULAR DYNAMICS SIMULATION OF NANOMETRIC CUTTING PROCESS. <i>International Journal of Nanoscience</i> , <b>2006</b> , 05, 633-638	0.6	1

7	STUDY ON NANOMETRIC CUTTING MECHANISM AND BURR FORMATION USING MOLECULAR DYNAMICS SIMULATION. <i>International Journal of Nanoscience</i> , <b>2006</b> , 05, 547-551	0.6	1
6	Thermo-Mechanical Modeling and Analysis of Equal Channel Angular Pressing. <i>Journal of Metastable and Nanocrystalline Materials</i> , <b>2005</b> , 23, 263-266	0.2	1
5	Modelling of Defects and Failure in 2D Materials: Graphene and Beyond <b>2020</b> , 1869-1909		1
4	Defect-Engineered Thermal Transport in Wrinkled Graphene: A Comprehensive Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , <b>2022</b> , 126, 5759-5766	3.8	1
3	Atomistic-scale analysis of the deformation and failure of polypropylene composites reinforced by functionalized silica nanoparticles. <i>Scientific Reports</i> , <b>2021</b> , 11, 23108	4.9	0
2	Modeling and Analysis of the Geometry-Dependent Mechanical and Thermal Properties of Coiled Carbon Nanotubes. <i>Physica Status Solidi - Rapid Research Letters</i> , 2100360	2.5	0
1	MECHANICAL PROPERTIES AND FRACTURE BEHAVIOR OF GRAPHENE AND OTHER 2D MATERIALS <b>2015</b> , 75-76		