

# Wei Kang

## List of Publications by Year in descending order

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63  
papers

2,482  
citations

361413

20  
h-index

197818

49  
g-index

64  
all docs

64  
docs citations

64  
times ranked

3760  
citing authors

#	ARTICLE	IF	CITATIONS
1	Finite-temperature phonon dispersion and vibrational dynamics of BaTiO <sub>3</sub> from first-principles molecular dynamics. <i>Physical Review B</i> , 2022, 105, .	3.2	3
2	Determination of concerted or stepwise mechanism of hydrogen tunneling from isotope effects: Departure between experiment and theory. <i>Journal of Chemical Physics</i> , 2022, 156, 124304.	3.0	4
3	First-Principles Study of the Structural, Electronic, and Enhanced Optical Properties of SnS <sub>2</sub> /TaS <sub>2</sub> Heterojunction. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 2177-2184.	8.0	5
4	Effect of High Order Phonon Scattering on the Thermal Conductivity and Its Response to Strain of a Penta-NiN <sub>2</sub> Sheet. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5734-5741.	4.6	16
5	Transition of the generation mechanism of high-order harmonics in an extended neon system. <i>Matter and Radiation at Extremes</i> , 2022, 7, 044403.	3.9	1
6	Dynamics of particles near the surface of a medium under ultra-strong shocks. <i>Matter and Radiation at Extremes</i> , 2021, 6, .	3.9	3
7	First-principles calculations of K-shell x-ray absorption spectra for warm dense ammonia*. <i>Chinese Physics B</i> , 2021, 30, 057102.	1.4	1
8	Equations of state of poly- $\alpha$ -methylstyrene and polystyrene: First-principles calculations versus precision measurements. <i>Physical Review B</i> , 2021, 103, .	3.2	8
9	Phonon Transport and Thermoelectric Properties of Imidazole-Graphyne. <i>Materials</i> , 2021, 14, 5604.	2.9	3
10	Boron-Functionalized Organic Framework as a High-Performance Metal-Free Catalyst for N <sub>2</sub> Fixation. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 12142-12149.	4.6	9
11	Dynamics of bond breaking and formation in polyethylene near shock front. <i>Physical Review E</i> , 2020, 102, 023207.	2.1	1
12	First-principles method for x-ray Thomson scattering including both elastic and inelastic features in warm dense matter. <i>Physical Review B</i> , 2020, 102, .	3.2	6
13	Stopping power of hot dense deuterium-tritium plasmas mixed with impurities to charged particles. <i>Physical Review E</i> , 2020, 101, 053209.	2.1	5
14	Temperature effect on the phase stability of hydrogen $\sqrt{2} \times \sqrt{2}$ phase from first-principles molecular dynamics calculations. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 405404.	1.8	3
15	Coupling effects and thin-shell corrections for surface instabilities of cylindrical fluid shells. <i>Physical Review E</i> , 2020, 101, 023108.	2.1	3
16	Inverting shock-wave temperatures via artificial neural networks. <i>Journal of Applied Physics</i> , 2020, 127, 125901.	2.5	1
17	High-energy-density physics based on HIAF. <i>Scientia Sinica: Physica, Mechanica Et Astronomica</i> , 2020, 50, 112004.	0.4	1
18	Measurement of ionic structure in isochorically heated graphite from X-ray Thomson scattering. <i>Physics of Plasmas</i> , 2019, 26, 022702.	1.9	1

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19	Nano-architected metamaterials: Carbon nanotube-based nanotrusses. Carbon, 2018, 131, 38-46.	10.3	29
20	Finite-temperature infrared and Raman spectra of high-pressure hydrogen from first-principles molecular dynamics. Physical Review B, 2018, 98, .	3.2	14
21	First-Principles Estimation of Electronic Temperature from X-Ray Thomson Scattering Spectrum of Isochorically Heated Warm Dense Matter. Physical Review Letters, 2018, 120, 205002.	7.8	20
22	Molecular dynamics simulation of strong shock waves propagating in dense deuterium, taking into consideration effects of excited electrons. Physical Review E, 2017, 95, 023201.	2.1	29
23	Theoretical study on electron-phonon coupling factor and electron-ion nonequilibrium process in uranium. Physics of Plasmas, 2017, 24, 022703.	1.9	2
24	X-ray absorption of liquid water by advanced <i>ab initio</i> methods. Physical Review B, 2017, 96, .	3.2	11
25	First-principles calculations of X-ray absorption spectra for warm dense methane. Physics of Plasmas, 2017, 24, 092705.	1.9	1
26	Recent progresses on numerical investigations of microscopic structure of strong shock waves in fluid. Scientia Sinica: Physica, Mechanica Et Astronomica, 2017, 47, 070003.	0.4	6
27	First-Principles Investigation to Ionization of Argon Under Conditions Close to Typical Sonoluminescence Experiments. Scientific Reports, 2016, 6, 20623.	3.3	8
28	Dynamic properties of the energy loss of multi-MeV charged particles traveling in two-component warm dense plasmas. Physical Review E, 2016, 94, 063203.	2.1	7
29	Extended application of Kohn-Sham first-principles molecular dynamics method with plane wave approximation at high energy-From cold materials to hot dense plasmas. Physics of Plasmas, 2016, 23, .	1.9	54
30	Electronic and optical properties of (U,Th)O <sub>2</sub> compound from screened hybrid density functional studies. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 1481-1486.	2.1	12
31	Molecular dynamics simulations of microscopic structure of ultra strong shock waves in dense helium. Frontiers of Physics, 2016, 11, 1.	5.0	28
32	Ferroelectricity and Phase Transitions in Monolayer Group-IV Monochalcogenides. Physical Review Letters, 2016, 117, 097601.	7.8	468
33	Thermal conductance of one-dimensional materials calculated with typical lattice models. Physical Review E, 2016, 94, 052131.	2.1	5
34	Link between $K$ -absorption edges and thermodynamic properties of warm dense plasmas established by an improved first-principles method. Physical Review B, 2016, 93, .	3.2	28
35	Validity boundary of orbital-free molecular dynamics method corresponding to thermal ionization of shell structure. Physical Review B, 2016, 94, .	3.2	20
36	First-principles calculations of K-shell X-ray absorption spectra for warm dense nitrogen. Physics of Plasmas, 2016, 23, 053304.	1.9	2

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37	Generalized Lenard-Balescu calculations of electron-ion temperature relaxation in beryllium plasma. <i>Physical Review E</i> , 2015, 92, 033103.	2.1	7
38	Transport properties of hydrogen-helium mixtures at extreme density and temperature conditions. <i>Physical Review E</i> , 2015, 92, 043108.	2.1	3
39	First-principles calculation of principal Hugoniot and K-shell X-ray absorption spectra for warm dense KCl. <i>Physics of Plasmas</i> , 2015, 22, 062707.	1.9	8
40	Temperature and compression effects on electron heat capacity and electron-phonon coupling in aluminum and beryllium: Insights from <i>ab initio</i> simulations. <i>Physics of Plasmas</i> , 2015, 22, .	1.9	8
41	Impact of isotopic disorders on thermal transport properties of nanotubes and nanowires. <i>Journal of Applied Physics</i> , 2015, 117, 035101.	2.5	1
42	H <sup>+</sup> (D <sup>+</sup> , T <sup>+</sup> ) beryllium collisions studied using time-dependent density functional theory. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015, 379, 319-326.	2.1	9
43	Comparison of electronic energy loss in graphene and BN sheet by means of time-dependent density functional theory. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 025401.	1.8	27
44	MXene nanoribbons. <i>Journal of Materials Chemistry C</i> , 2015, 3, 879-888.	5.5	65
45	Ubiquitous thermal rectification induced by non-diffusive weak scattering at low temperature in one-dimensional materials: Revealed with a non-reflective heat reservoir. <i>Europhysics Letters</i> , 2014, 105, 16004.	2.0	12
46	Manipulation of electronic and magnetic properties of M <sub>2</sub> C (M = Hf, Nb, Sc, Ta, Ti, V, Zr) monolayer by applying mechanical strains. <i>Applied Physics Letters</i> , 2014, 104, .	3.3	139
47	Gas adsorption on MoS <sub>2</sub> monolayer from first-principles calculations. <i>Chemical Physics Letters</i> , 2014, 595-596, 35-42.	2.6	328
48	Parameterizing the Morse potential for coarse-grained modeling of blood plasma. <i>Journal of Computational Physics</i> , 2014, 257, 726-736.	3.8	19
49	The potential application of phosphorene as an anode material in Li-ion batteries. <i>Journal of Materials Chemistry A</i> , 2014, 2, 19046-19052.	10.3	339
50	Heat transfer in heterogeneous nanostructures can be described by a simple chain model. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16914-16918.	2.8	5
51	Role of Strain and Concentration on the Li Adsorption and Diffusion Properties on Ti <sub>2</sub> C Layer. <i>Journal of Physical Chemistry C</i> , 2014, 118, 14983-14990.	3.1	88
52	Design of Medium Band Gap AgBiNbO and AgBiTaO Semiconductors for Driving Direct Water Splitting with Visible Light. <i>Inorganic Chemistry</i> , 2013, 52, 9192-9205.	4.0	9
53	Electronic structure and quasiparticle bandgap of silicene structures. <i>Applied Physics Letters</i> , 2013, 102, .	3.3	79
54	Ion selection of charge-modified large nanopores in a graphene sheet. <i>Journal of Chemical Physics</i> , 2013, 139, 114702.	3.0	95

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55	Van der Waals interaction-tuned heat transfer in nanostructures. <i>Nanoscale</i> , 2013, 5, 128-133.	5.6	29
56	Antiferromagnetic FeSe monolayer on SrTiO3: The charge doping and electric field effects. <i>Scientific Reports</i> , 2013, 3, 2213.	3.3	64
57	Viscous flow simulation in a stenosis model using discrete particle dynamics: a comparison between DPD and CFD. <i>Biomechanics and Modeling in Mechanobiology</i> , 2012, 11, 119-129.	2.8	24
58	Enhanced static approximation to the electron self-energy operator for efficient calculation of quasiparticle energies. <i>Physical Review B</i> , 2010, 82, .	3.2	42
59	Quasiparticle and optical properties of rutile and anatase $\text{TiO}_2$ <i>Physical Review B</i> , 2010, 82, .	3.2	192
60	Thermal bending of nanojets: Molecular dynamics simulations of an asymmetrically heated nozzle. <i>Applied Physics Letters</i> , 2008, 93, .	3.3	15
61	Universality Crossover of the Pinch-Off Shape Profiles of Collapsing Liquid Nanobridges in Vacuum and Gaseous Environments. <i>Physical Review Letters</i> , 2007, 98, 064504.	7.8	46
62	Thermodynamic second law in irreversible processes of chaotic few-body systems. <i>Physical Review E</i> , 2001, 64, 045102.	2.1	4
63	Chaoslike behavior in nonchaotic systems at finite computation precision. <i>Physical Review E</i> , 2001, 63, 046310.	2.1	7