

# Jiayu Dai

## List of Publications by Year in descending order

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58  
papers

1,794  
citations

430442

18  
h-index

276539

41  
g-index

59  
all docs

59  
docs citations

59  
times ranked

2196  
citing authors

#	ARTICLE	IF	CITATIONS
1	Gas adsorption on graphene doped with B, N, Al, and S: A theoretical study. Applied Physics Letters, 2009, 95, .	1.5	643
2	Adsorption of molecular oxygen on doped graphene: Atomic, electronic, and magnetic properties. Physical Review B, 2010, 81, .	1.1	232
3	Modulating the electronic and magnetic structures of P-doped graphene by molecule doping. Journal of Physics Condensed Matter, 2010, 22, 225501.	0.7	75
4	Electronic structure tuning and band gap opening of graphene by hole/electron codoping. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 3890-3894.	0.9	71
5	Unified First Principles Description from Warm Dense Matter to Ideal Ionized Gas Plasma: Electron-Ion Collisions Induced Friction. Physical Review Letters, 2010, 104, 245001.	2.9	58
6	<i>Ab initio</i> study of pressure-driven phase transition in $\text{FePS}_3$ and $\text{FePSe}_3$ . Physical Review B, 2019, 100, .	1.1	42
7	Large-scale efficient Langevin dynamics, and why it works. Europhysics Letters, 2009, 88, 20001.	0.7	40
8	Light-induced irreversible structural phase transition in trilayer graphene. Light: Science and Applications, 2020, 9, 174.	7.7	40
9	Structure and vibrational spectra of small water clusters from first principles simulations. Journal of Chemical Physics, 2010, 133, 014302.	1.2	39
10	Changes of structure and dipole moment of water with temperature and pressure: A first principles study. Journal of Chemical Physics, 2011, 135, 024505.	1.2	38
11	Dynamic Ionic Clusters with Flowing Electron Bubbles from Warm to Hot Dense Iron along the Hugoniot Curve. Physical Review Letters, 2012, 109, 175701.	2.9	32
12	Extremely Low Electron-ion Temperature Relaxation Rates in Warm Dense Hydrogen: Interplay between Quantum Electrons and Coupled Ions. Physical Review Letters, 2019, 122, 015001.	2.9	31
13	Structure, equation of state, diffusion and viscosity of warm dense Fe under the conditions of a giant planet core. New Journal of Physics, 2013, 15, 045003.	1.2	29
14	Quantum simulation of thermally-driven phase transition and oxygen K-edge x-ray absorption of high-pressure ice. Scientific Reports, 2013, 3, 3272.	1.6	26
15	QUANTUM LANGEVIN MOLECULAR DYNAMIC DETERMINATION OF THE SOLAR-INTERIOR EQUATION OF STATE. Astrophysical Journal, 2010, 721, 1158-1163.	1.6	23
16	Physisorption to chemisorption transition of NO <sub>2</sub> on graphene induced by the interplay of SiO <sub>2</sub> substrate and van der Waals forces: A first principles study. Chemical Physics, 2012, 405, 161-166.	0.9	23
17	Nuclear quantum dynamics in dense hydrogen. Scientific Reports, 2014, 4, 5484.	1.6	20
18	Dynamic electron-ion collisions and nuclear quantum effects in quantum simulation of warm dense matter. Journal of Physics Condensed Matter, 2018, 30, 073002.	0.7	18

#	ARTICLE	IF	CITATIONS
19	Extreme nonlinear strong-field photoemission from carbon nanotubes. <i>Nature Communications</i> , 2019, 10, 4891.	5.8	16
20	Towards the Same Line of Liquid–Liquid Phase Transition of Dense Hydrogen from Various Theoretical Predictions. <i>Chinese Physics Letters</i> , 2019, 36, 103102.	1.3	15
21	First-principles study on equation of states and electronic structures of shock compressed Ar up to warm dense regime. <i>Journal of Chemical Physics</i> , 2016, 144, 124503.	1.2	14
22	Ab initio validation on the connection between atomistic and hydrodynamic description to unravel the ion dynamics of warm dense matter. <i>Physical Review Research</i> , 2021, 3, .	1.3	14
23	Achieving a direct band gap and high power conversion efficiency in an $SbI_3/BiI_3$ type-II vdW heterostructure via interlayer compression and electric field application. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2619-2627.	1.3	13
24	Molecular dynamics simulation of electron–ion temperature relaxation in dense hydrogen: A scheme of truncated Coulomb potential. <i>High Energy Density Physics</i> , 2014, 13, 34-39.	0.4	12
25	Phase-Changing in Graphite Assisted by Interface Charge Injection. <i>Nano Letters</i> , 2021, 21, 5648-5654.	4.5	12
26	Multishock compression of dense cryogenic hydrogen-helium mixtures up to 60 GPa: Validating the equation of state calculated from first principles. <i>Physical Review B</i> , 2018, 98, .	1.1	11
27	Quantum molecular dynamics study on the structures and dc conductivity of warm dense silane. <i>Physical Review E</i> , 2014, 89, 022128.	0.8	10
28	Directly calculated electrical conductivity of hot dense hydrogen from molecular dynamics simulation beyond Kubo-Greenwood formula. <i>Physics of Plasmas</i> , 2018, 25, .	0.7	10
29	Unified first-principles equations of state of deuterium-tritium mixtures in the global inertial confinement fusion region. <i>Matter and Radiation at Extremes</i> , 2020, 5, .	1.5	10
30	Structural transition dynamics of the formation of warm dense gold: From an atomic scale view. <i>Science China: Physics, Mechanics and Astronomy</i> , 2020, 63, 1.	2.0	10
31	Toward accurate electronic, optical, and vibrational properties of hexagonal Si, Ge, and $Si_1-xGe_x$ alloys from first-principle simulations. <i>Journal of Applied Physics</i> , 2021, 129, .	1.1	10
32	Strong bulk-surface interaction dominated in-plane anisotropy of electronic structure in GaTe. <i>Communications Physics</i> , 2022, 5, .	2.0	10
33	Influence of ordered structures on electrical conductivity and XANES from warm to hot dense matter. <i>High Energy Density Physics</i> , 2011, 7, 84-90.	0.4	9
34	Equations of state and transport properties of mixtures in the warm dense regime. <i>Physics of Plasmas</i> , 2015, 22, .	0.7	9
35	Benchmarking the diffusion and viscosity of H-He mixtures in warm dense matter regime by quantum molecular dynamics simulations. <i>Physics of Plasmas</i> , 2017, 24, .	0.7	9
36	Direct Visualization and Manipulation of Stacking Orders in Few-Layer Graphene by Dynamic Atomic Force Microscopy. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7328-7334.	2.1	9

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37	Temperature dependence of adsorption and desorption dynamics of NO <sub>2</sub> molecule on boron-doped graphene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 137, 115083.	1.3	9
38	Quantum molecular dynamics study on the proton exchange, ionic structures, and transport properties of warm dense hydrogen-deuterium mixtures. <i>Physical Review E</i> , 2018, 97, 063204.	0.8	8
39	Benchmarking the effective one-component plasma model for warm dense neon and krypton within quantum molecular dynamics simulation. <i>Physical Review E</i> , 2020, 101, 023302.	0.8	8
40	Towards large-scale and spatiotemporally resolved diagnosis of electronic density of states by deep learning. <i>Physical Review B</i> , 2022, 105, .	1.1	8
41	Temperature-dependent vibrational spectra and melting behavior of small silicon clusters based on <i>ab initio</i> molecular dynamics simulations. <i>Physical Review A</i> , 2009, 79, .	1.0	7
42	Stability and local magnetic moment of bilayer graphene by intercalation: first principles study. <i>RSC Advances</i> , 2018, 8, 19732-19738.	1.7	7
43	The effect of external temperature gradients on thermal conductivity in non-equilibrium molecular dynamics simulations: From nanowires to bulk Si. <i>Journal of Chemical Physics</i> , 2019, 151, 064116.	1.2	6
44	Multishock to Quasi-Isentropic Compression of Dense Gaseous Deuterium-Helium Mixtures up to 120 ÅGPa: Probing the Sound Velocities Relevant to Planetary Interiors. <i>Physical Review Letters</i> , 2021, 126, 075701.	2.9	6
45	Reduced ionic diffusion by the dynamic electron-ion collisions in warm dense hydrogen. <i>Physics of Plasmas</i> , 2021, 28, 012704.	0.7	6
46	Finite-temperature density-functional-theory investigation on the nonequilibrium transient warm-dense-matter state created by laser excitation. <i>Physical Review E</i> , 2021, 103, 013210.	0.8	6
47	Optical-Field-Driven Electron Tunneling in Metal-Insulator-Metal Nanojunction. <i>Advanced Science</i> , 2021, , 2101572.	5.6	6
48	Plasmonic evolution of atomically size-selected Au clusters by electron energy loss spectrum. <i>National Science Review</i> , 2020, 8, nwaa282.	4.6	5
49	Electronic and optical properties of warm dense lithium: strong coupling effects. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2017, 50, 184004.	0.6	4
50	Molecular dynamics investigation of the stopping power of warm dense hydrogen for electrons. <i>Physical Review E</i> , 2021, 103, 063215.	0.8	4
51	<i>Ab initio</i> study of the miscibility for solid hydrogen-helium mixtures at high pressure. <i>Journal of Chemical Physics</i> , 2020, 152, 074701.	1.2	3
52	Bound electron screening effect on ion-ion potential of warm and hot dense matter. <i>Physical Review E</i> , 2021, 103, L051203.	0.8	3
53	Doping-controllable high temperature magnetic semiconductor. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 131, 114731.	1.3	3
54	Nanoscale Topological Morphology Transition and Controllable Thermal Conductivity of Wrinkled Hexagonal Boron Nitride: Implications for Thermal Manipulation and Management. <i>ACS Applied Nano Materials</i> , 0, , .	2.4	3

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55	Enhanced pair production in collisions of intense pulsed lasers with a high-energy electron beam. <i>Physical Review A</i> , 2019, 100, .	1.0	2
56	Controlled Epitaxial Growth and Atomically Sharp Interface of Graphene/Ferromagnetic Heterostructure via Ambient Pressure Chemical Vapor Deposition. <i>Nanomaterials</i> , 2021, 11, 3112.	1.9	2
57	Reduced graphene oxide spatially scaffolded by a sucrose-derived carbon framework for trace and fast gas detection. <i>Carbon</i> , 2022, 191, 164-174.	5.4	2
58	Effect of Nonequilibrium Transient Electronic Structures on Lattice Stability in Metals: Density Functional Theory Calculations. <i>Frontiers in Physics</i> , 2022, 10, .	1.0	1