Peitao Liu

List of Publications by Year
in descending order

35 papers	1,173 citations	393982 19 h-index	377514 34 g-index
35 all docs	35 docs citations	35 times ranked	1610 citing authors

#	Article	IF	Citations
1	Extra-electron induced covalent strengthening and generalization of intrinsic ductile-to-brittle criterion. Scientific Reports, 2012, 2, 718.	1.6	165
2	Cubic scaling<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m Towards fast quasiparticle calculations. Physical Review B, 2016, 94, .	1.1	113
3	GW100: A Plane Wave Perspective for Small Molecules. Journal of Chemical Theory and Computation, 2017, 13, 635-648.	2.3	74
4	Interstitial-boron solution strengthened WB3+x. Applied Physics Letters, 2013, 103, .	1.5	72
5	Anisotropic magnetic couplings and structure-driven canted to collinear transitions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn> magnetically constrained noncollinear DFT. Physical Review B, 2015, 92, .	1.1	70
6	Thermal transport and phase transitions of zirconia by on-the-fly machine-learned interatomic potentials. Npj Computational Materials, 2021, 7, .	3.5	57
7	Beyond the quasiparticle approximation: Fully self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow> calculations. Physical Review B, 2018, 98, .	1.1	56
8	Merging GW with DMFT and non-local correlations beyond. European Physical Journal: Special Topics, 2017, 226, 2565-2590.	1.2	45
9	Converged <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow> quasiparticle energies for transition metal oxide perovskites. Physical Review Materials, 2018, 2, .	0.9	45
10	Relativistic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow> +BSE study of the optical properties of Ruddlesden-Popper iridates. Physical Review Materials, 2018, 2, .	0.9	40
11	Effects of dilute substitutional solutes on interstitial carbon in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math>-Fe: Interactions and associated carbon diffusion from first-principles calculations. Physical Review B, 2014, 90, .	1.1	38
12	Dimensionality-strain phase diagram of strontium iridates. Physical Review B, 2017, 95, .	1.1	37
13	Lifshitz transition driven by spin fluctuations and spin-orbit renormalization inNaOsO3. Physical Review B, 2016, 94, .	1.1	34
14	Assessing model-dielectric-dependent hybrid functionals on the antiferromagnetic transition-metal monoxides MnO, FeO, CoO, and NiO. Journal of Physics Condensed Matter, 2020, 32, 015502.	0.7	30
15	Accurate optical spectra through time-dependent density functional theory based on screening-dependent hybrid functionals. Physical Review Research, 2020, 2, .	1.3	29
16	Energetics of the coupled electronicâ€“structural transition in the rare-earth nickelates. Npj Quantum Materials, 2019, 4, .	1.8	28
17	Electron and hole doping in the relativistic Mott insulator <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Sr</mml:mi><mml:mn mathvariant="bold">2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">IrO</mml:mi><mml:mn	1.1	27
18	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi><mml:mtext>â€™</mml:mtext><mml:mi>Î²</mml:mi></mml:mrow> phase transition of zirconium predicted by on-the-fly machine-learned force field. Physical Review Materials, 2021, 5, .	0.9	21

#	Article	IF	Citations
19	Phase transitions of zirconia: Machine-learned force fields beyond density functional theory. Physical Review B, 2022, 105, .	1.1	21
20	Fast and Huge Anisotropic Diffusion of Cu (Ag) and Its Resistance on the Sn Self-diffusivity in Solid Î²â€“Sn. Journal of Materials Science and Technology, 2016, 32, 121-128.	5.6	18
21	Strain-induced tuning of the electronic Coulomb interaction in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math> transition metal oxide perovskites. Physical Review B, 2018, 98, .	1.1	18
22	Tunable relativistic quasiparticle electronic and excitonic behavior of the FAPb(I_{1â^'x}Br_x)₃ alloy. Physical Chemistry Chemical Physics, 2020, 22, 11943-11955.	1.3	18
23	Vacancy formation enthalpy of filled<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math>-band noble metals by hybrid functionals. Physical Review B, 2014, 90, .	1.1	15
24	Magnetic properties of bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Sr</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Ir</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> : Role of interplay between multipolar spin interactions, Jahn-Teller effect, and electronic correlation in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>J</mml:mi><mml:mtext>eff</mml:mtext></mml:msub></mml:mrow></mml:math> insulator. Physical Review B, 2021, 103, .	1.1	15
25		1.1	14
26	Kagome metal-organic frameworks as a platform for strongly correlated electrons. JPhys Materials, 2020, 3, 025001.	1.8	11
27	Comparative ab initio study of the structural, electronic, magnetic, and dynamical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiOsO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>NaOsO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>	0.9	11
28	Osmates on the Verge of a Hundâ€™s-Mott Transition: The Different Fates of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NaOsO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>LiOsO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Letters, 2020, 125, 166402.	2.9	10
29	Cubic and tetragonal perovskites from the random phase approximation. Physical Review Materials, 2019, 3, .	0.9	10
30	Optical and excitonic properties of transition metal oxide perovskites by the Bethe-Salpeter equation. Physical Review Materials, 2021, 5, .	0.9	9
31	First-principles studies of hydrogen behavior interacting with oxygen-enriched nanostructured particles in the ODS steels. International Journal of Hydrogen Energy, 2014, 39, 18506-18519.	3.8	7
32	Advanced First-Principle Modeling of Relativistic Ruddlesdenâ€”Popper Strontium Iridates. Applied Sciences (Switzerland), 2021, 11, 2527.	1.3	5
33	Aberrant electronic and structural alterations in pressure tuned perovskite NaOsO3. Npj Quantum Materials, 2020, 5, .	1.8	4
34	Nanoscale synthesis of ionic analogues of bilayer silicene with high carrier mobility. Journal of Materials Chemistry C, 2021, 9, 8545-8551.	2.7	4
35	Revealing the quasiparticle electronic and excitonic nature in cubic, tetragonal, and hexagonal phases of FAPbI₃. AIP Advances, 2022, 12, 025330.	0.6	2