Peitao Liu

List of Publications by Citations

33 papers	736 citations	15 h-index	26 g-index
35 ext. papers	968 ext. citations	4.1 avg, IF	4.31 L-index

#	Paper	IF	Citations
33	Extra-electron induced covalent strengthening and generalization of intrinsic ductile-to-brittle criterion. *Scientific Reports*, **2012**, 2, 718	4.9	123
32	Cubic scaling GW: Towards fast quasiparticle calculations. *Physical Review B*, **2016**, 94,	3.3	74
31	Interstitial-boron solution strengthened WB3+x. *Applied Physics Letters*, **2013**, 103, 171903	3.4	62
30	GW100: A Plane Wave Perspective for Small Molecules. *Journal of Chemical Theory and Computation* , **2017**, 13, 635-648	6.4	58
29	Anisotropic magnetic couplings and structure-driven canted to collinear transitions in Sr2IrO4 by magnetically constrained noncollinear DFT. *Physical Review B*, **2015**, 92,	3.3	55
28	Effects of dilute substitutional solutes on interstitial carbon in □Fe: Interactions and associated carbon diffusion from first-principles calculations. *Physical Review B*, **2014**, 90,	3.3	35
27	Beyond the quasiparticle approximation: Fully self-consistent GW calculations. *Physical Review B*, **2018**, 98,	3.3	35
26	Merging GW with DMFT and non-local correlations beyond. *European Physical Journal: Special Topics* , **2017**, 226, 2565-2590	2.3	30
25	Converged GW quasiparticle energies for transition metal oxide perovskites. *Physical Review Materials*, **2018**, 2,	3.2	28
24	Lifshitz transition driven by spin fluctuations and spin-orbit renormalization in NaOsO3. *Physical Review B*, **2016**, 94,	3.3	27
23	Dimensionality-strain phase diagram of strontium iridates. *Physical Review B*, **2017**, 95,	3.3	26
22	Relativistic GW+BSE study of the optical properties of Ruddlesden-Popper iridates. *Physical Review Materials*, **2018**, 2,	3.2	23
21	Electron and hole doping in the relativistic Mott insulator Sr2IrO4: A first-principles study using band unfolding technique. *Physical Review B*, **2016**, 94,	3.3	23
20	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	1.8	16
19	Energetics of the coupled electronic□tructural transition in the rare-earth nickelates. *Npj Quantum Materials*, **2019**, 4,	5	15
18	Magnetic properties of bilayer Sr3Ir2O7: Role of epitaxial strain and oxygen vacancies. *Physical Review B*, **2017**, 95,	3.3	12
17	Vacancy formation enthalpy of filled d-band noble metals by hybrid functionals. *Physical Review B*, **2014**, 90,	3.3	12

16	Accurate optical spectra through time-dependent density functional theory based on screening-dependent hybrid functionals. *Physical Review Research*, **2020**, 2,	3.9	11
15	Tunable relativistic quasiparticle electronic and excitonic behavior of the FAPb(IBr) alloy. *Physical Chemistry Chemical Physics*, **2020**, 22, 11943-11955	3.6	10
14	Fast and Huge Anisotropic Diffusion of Cu (Ag) and Its Resistance on the Sn Self-diffusivity in Solid β-Sn. *Journal of Materials Science and Technology*, **2016**, 32, 121-128	9.1	10
13	Strain-induced tuning of the electronic Coulomb interaction in 3d transition metal oxide perovskites. *Physical Review B*, **2018**, 98,	3.3	10
12	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	6.7	6
11	Cubic and tetragonal perovskites from the random phase approximation. *Physical Review Materials*, **2019**, 3,	3.2	6
10	Thermal transport and phase transitions of zirconia by on-the-fly machine-learned interatomic potentials. *Npj Computational Materials*, **2021**, 7,	10.9	6
9	Comparative ab initio study of the structural, electronic, magnetic, and dynamical properties of LiOsO3 and NaOsO3. *Physical Review Materials*, **2020**, 4,	3.2	5
8	Osmates on the Verge of a Hund-Mott Transition: The Different Fates of NaOsO_{3} and LiOsO_{3}. *Physical Review Letters*, **2020**, 125, 166402	7.4	5
7	Kagome metal-organic frameworks as a platform for strongly correlated electrons. *JPhys Materials*, **2020**, 3, 025001	4.2	2
6	Ωphase transition of zirconium predicted by on-the-fly machine-learned force field. *Physical Review Materials*, **2021**, 5,	3.2	2
5	Nanoscale synthesis of ionic analogues of bilayer silicene with high carrier mobility. *Journal of Materials Chemistry C*, **2021**, 9, 8545-8551	7.1	2
4	Aberrant electronic and structural alterations in pressure tuned perovskite NaOsO3. *Npj Quantum Materials*, **2020**, 5,	5	1
3	Interplay between multipolar spin interactions, Jahn-Teller effect, and electronic correlation in a Jeff=32 insulator. *Physical Review B*, **2021**, 103,	3.3	1
2	Advanced First-Principle Modeling of Relativistic Ruddlesden-Popper Strontium Iridates. *Applied Sciences (Switzerland)*, **2021**, 11, 2527	2.6	1
1	Revealing the quasiparticle electronic and excitonic nature in cubic, tetragonal, and hexagonal phases of FAPbI3. *AIP Advances*, **2022**, 12, 025330	1.5	