Phil Hasnip

List of Publications by Year
in descending order

36	19,892	567144 15	360920 35
papers	citations	h-index	g-index

37	37	37	16839
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First principles methods using CASTEP. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	9,458
2	First-principles simulation: ideas, illustrations and the CASTEP code. Journal of Physics Condensed Matter, 2002, 14, 2717-2744.	0.7	8,382
3	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
4	Density functional theory in the solid state. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130270.	1.6	242
5	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
6	Electronic energy minimisation with ultrasoft pseudopotentials. Computer Physics Communications, 2006, 174, 24-29.	3.0	86
7	Computing the self-consistent field in Kohnâ€“Sham density functional theory. Journal of Physics Condensed Matter, 2019, 31, 453001.	0.7	38
8	Ab initio studies of disorder in the full Heusler alloy Co2FexMn1â^'xSi. Journal of Applied Physics, 2013, 113, .	1.1	36
9	Huge power factor in p-type half-Heusler alloys NbFeSb and TaFeSb. JPhys Materials, 2019, 2, 035002.	1.8	33
10	Exchange coupling and magnetic anisotropy at Fe/FePt interfaces. Physical Review B, 2013, 88, .	1.1	31
11	DL_MG: A Parallel Multigrid Poisson and Poissonâ€“Boltzmann Solver for Electronic Structure Calculations in Vacuum and Solution. Journal of Chemical Theory and Computation, 2018, 14, 1412-1432.	2.3	31
12	Dynamically Stabilized Growth of Polar Oxides: The Case of MgO(111). Physical Review Letters, 2011, 107, 056101.	2.9	27
13	Many-body renormalization of forces in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>f</mml:mi></mml:math> -electron materials. Physical Review B, 2018, 98, .	1.1	20
14	Realisation of magnetically and atomically abrupt half-metal/semiconductor interface: Co2FeSi0.5Al0.5/Ge(111). Scientific Reports, 2016, 6, 37282.	1.6	18
15	The role of chemical structure on the magnetic and electronic properties of Co2FeAl0.5Si0.5/Si(111) interface. Applied Physics Letters, 2016, 108, .	1.5	15
16	Correlation between spin transport signal and Heusler/semiconductor interface quality in lateral spin-valve devices. Physical Review B, 2018, 98, .	1.1	15
17	The effect of film and interface structure on the transport properties of Heusler based current-perpendicular-to-plane spin valves. Applied Physics Letters, 2011, 98, .	1.5	14
18	Experimental and density functional study of Mn doped Bi2Te3 topological insulator. APL Materials, 2016, 4, .	2.2	14

#	Article	IF	Citations
19	The effect of atomic structure on interface spin-polarization of half-metallic spin valves: Co2MnSi/Ag epitaxial interfaces. Applied Physics Letters, 2015, 107, .	1.5	13
20	Off-the-shelf DFT-DISPersion methods: Are they now â€œon-trendâ€•for organic molecular crystals?. Journal of Chemical Physics, 2019, 151, 044106.	1.2	11
21	Structure of naturally hydrated ferrihydrite revealed through neutron diffraction and first-principles modeling. Physical Review Materials, 2017, 1, .	0.9	11
22	Growth and interface phase stability of barium hexaferrite films on SiC(0001). Journal of Applied Physics, 2011, 109, 07E520.	1.1	9
23	Tailoring the electrical properties of Ge/GaAs by film deposition rate and preparation of fully compensated Ge films. Physical Review B, 2011, 84, .	1.1	9
24	The Effect of Cobalt-Sublattice Disorder on Spin Polarisation in Co2FexMn1â^'xSi Heusler Alloys. Materials, 2014, 7, 1473-1482.	1.3	9
25	Simultaneous Prediction of the Magnetic and Crystal Structure of Materials Using a Genetic Algorithm. Crystals, 2019, 9, 439.	1.0	8
26	Correlations between atomic structure and giant magnetoresistance ratio in Co₂(Fe,Mn)Si spin valves. Journal Physics D: Applied Physics, 2014, 47, 322003.	1.3	7
27	Materials and Molecular Modeling at the Exascale. Computing in Science and Engineering, 2022, 24, 36-45.	1.2	7
28	Theoretical study of core-loss electron energy-loss spectroscopy at graphene nanoribbon edges. Journal of Physics Condensed Matter, 2015, 27, 305301.	0.7	5
29	Electronâ€“phonon interaction and superconductivity in hexagonal ternary carbides Nb₂AC (A: Al, S, Ge, As and Sn). Electronic Structure, 2021, 3, 045001.	1.0	5
30	Effective modelling of the Seebeck coefficient of Fe₂VAl. Journal of Physics Condensed Matter, 2020, 32, 125401.	0.7	4
31	Modification of the van der Waals interaction at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and Ge(111) interface. Physical Review Materials, 2021, 5, .	2.9	4
32	Portable Acceleration of Materials Modeling Software: CASTEP, GPUs, and OpenACC. Computing in Science and Engineering, 2022, 24, 46-55.	1.2	4
33	The effect of MgO(111) interlayer on the interface phase stability and structure of BaFe12O19/SiC(0001). Journal of Applied Physics, 2012, 111, 07A515.	1.1	3
34	Controlling the half-metallicity of Heusler/Si(1â€‰1â€‰1) interfaces by a monolayer of Siâ€“Coâ€“Si. Journal of Physics Condensed Matter, 2016, 28, 395003.	0.7	3
35	Significant improvement of the Seebeck coefficient of Fe2VAlÂwith antisite defects. Materials Today Communications, 2022, 31, 103510.	0.9	2
36	A fast, stable method for density functional simulations of nanostructures. Journal of Physics: Conference Series, 2011, 286, 012034.	0.3	0