

Martijn Marsman

List of Publications by Year in descending order

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33
papers

7,363
citations

304368

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377514

34
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36
all docs

36
docs citations

36
times ranked

8625
citing authors

#	ARTICLE	IF	CITATIONS
1	Screened hybrid density functionals applied to solids. Journal of Chemical Physics, 2006, 124, 154709.	1.2	1,915
2	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
3	The Perdew-Burke-Ernzerhof exchange-correlation functional applied to the G2-1 test set using a plane-wave basis set. Journal of Chemical Physics, 2005, 122, 234102.	1.2	754
4	Accurate Quasiparticle Spectra from Self-Consistent GW Calculations with Vertex Corrections. Physical Review Letters, 2007, 99, 246403.	2.9	606
5	Hybrid functionals applied to extended systems. Journal of Physics Condensed Matter, 2008, 20, 064201.	0.7	500
6	Why does the B3LYP hybrid functional fail for metals?. Journal of Chemical Physics, 2007, 127, 024103.	1.2	481
7	Making the random phase approximation to electronic correlation accurate. Journal of Chemical Physics, 2009, 131, 154115.	1.2	227
8	Second-order Møller-Plesset perturbation theory applied to extended systems. I. Within the projector-augmented-wave formalism using a plane wave basis set. Journal of Chemical Physics, 2009, 130, 184103.	1.2	194
9	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. Physical Review B, 2011, 84, .	1.1	180
10	Second-order Møller-Plesset perturbation theory applied to extended systems. II. Structural and energetic properties. Journal of Chemical Physics, 2010, 133, 074107.	1.2	147
11	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. Journal of Chemical Theory and Computation, 2011, 7, 2780-2785.	2.3	117
12	Relaxed core projector-augmented-wave method. Journal of Chemical Physics, 2006, 125, 104101.	1.2	112
13	Hyperfine coupling of point defects in semiconductors by hybrid density functional calculations: The role of core spin polarization. Physical Review B, 2013, 88, .	1.1	79
14	Anisotropic magnetic couplings and structure-driven canted to collinear transitions in Sr_2FeMoO_6 magnetically constrained noncollinear DFT. Physical Review B, 2015, 92, .		
15	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. Physical Review B, 2011, 83, .	1.1	67
16	Structural, electronic and magnetic properties of Gd investigated by DFT+U methods: bulk, clean and H-covered (0001) surfaces. Journal of Physics Condensed Matter, 2006, 18, 7021-7043.	0.7	64
17	Iron as a source of efficient Shockley-Read-Hall recombination in GaN. Applied Physics Letters, 2016, 109, .	1.5	64
18	Optical and electronic properties of SiN_4 and SiO_2 . Physical Review B, 2011, 83, .	1.1	57

#	ARTICLE	IF	CITATIONS
19	Charge self-consistent many-body corrections using optimized projected localized orbitals. Journal of Physics Condensed Matter, 2018, 30, 475901.	0.7	36
20	Density functional theory study of the structural and electronic properties of amorphous silicon nitrides: Si ₃ N ₄ . Physical Review B, 2012, 86, .	1.1	34
21	Magnetic doping of 4d transition-metal surfaces: A first-principles study. Physical Review B, 2005, 71, .	1.1	19
22	Defects and defect healing in amorphous Si ₃ N ₄ . Physical Review B, 2012, 86, .	1.1	19
23	Embedding for bulk systems using localized atomic orbitals. Journal of Chemical Physics, 2017, 147, 034110.	1.2	17
24	NMR shieldings from density functional perturbation theory: GIPAW versus all-electron calculations. Journal of Chemical Physics, 2017, 146, 064115.	1.2	15
25	OpenMP in VASP: Threading and SIMD. International Journal of Quantum Chemistry, 2019, 119, e25851.	1.0	15
26	Finite-field implementation of NMR chemical shieldings for molecules: Direct and converse gauge-including projector-augmented-wave methods. Journal of Chemical Physics, 2013, 139, 014109.	1.2	13
27	Electron-phonon interactions using the projector augmented-wave method and Wannier functions. Physical Review B, 2020, 101, .	1.1	10
28	Nonlinear behavior of the band gap of Pb _{1-x} Sn _x . Physical Review B, 2012, 86, .		