Martijn Marsman

List of Publications by Citations

35 papers	5,974 citations	21 h-index	36 g-index
36 ext. papers	6,695 ext. citations	4.4 avg, IF	5.43 L-index

#	Paper	IF	Citations
35	Screened hybrid density functionals applied to solids. *Journal of Chemical Physics*, **2006**, 124, 154709	3.9	1591
34	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
33	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	3.9	560
32	Accurate quasiparticle spectra from self-consistent GW calculations with vertex corrections. *Physical Review Letters*, **2007**, 99, 246403	7.4	529
31	Hybrid functionals applied to extended systems. *Journal of Physics Condensed Matter*, **2008**, 20, 064201	1.8	430
30	Why does the B3LYP hybrid functional fail for metals?. *Journal of Chemical Physics*, **2007**, 127, 024103	3.9	424
29	Making the random phase approximation to electronic correlation accurate. *Journal of Chemical Physics*, **2009**, 131, 154115	3.9	199
28	Second-order M□ller-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	3.9	167
27	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. *Physical Review B*, **2011**, 84,	3.3	138
26	Second-order M□ller-Plesset perturbation theory applied to extended systems. II. Structural and energetic properties. *Journal of Chemical Physics*, **2010**, 133, 074107	3.9	125
25	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. *Journal of Chemical Theory and Computation*, **2011**, 7, 2780-5	6.4	95
24	Relaxed core projector-augmented-wave method. *Journal of Chemical Physics*, **2006**, 125, 104101	3.9	93
23	Hyperfine coupling of point defects in semiconductors by hybrid density functional calculations: The role of core spin polarization. *Physical Review B*, **2013**, 88,	3.3	61
22	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. *Physical Review B*, **2011**, 83,	3.3	59
21	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
20	Structural, electronic and magnetic properties of Gd investigated by DFT+Umethods: bulk, clean and H-covered (0001) surfaces. *Journal of Physics Condensed Matter*, **2006**, 18, 7021-7043	1.8	51
19	Optical and electronic properties of Si3N4 and □SiO2. *Physical Review B*, **2012**, 85,	3.3	50

18	Electric Control of Magnetization and Interplay between Orbital Ordering and Ferroelectricity in a Multiferroic Metal□Organic Framework. *Angewandte Chemie*, **2011**, 123, 5969-5972	3.6	50
17	Iron as a source of efficient Shockley-Read-Hall recombination in GaN. *Applied Physics Letters*, **2016**, 109, 162107	3.4	50
16	Density functional theory study of the structural and electronic properties of amorphous silicon nitrides: Si3N4□:H. *Physical Review B*, **2012**, 86,	3.3	23
15	Magnetic doping of 4d transition-metal surfaces: A first-principles study. *Physical Review B*, **2005**, 71,	3.3	19
14	Embedding for bulk systems using localized atomic orbitals. *Journal of Chemical Physics*, **2017**, 147, 034110	3.9	16
13	Charge self-consistent many-body corrections using optimized projected localized orbitals. *Journal of Physics Condensed Matter*, **2018**, 30, 475901	1.8	16
12	Defects and defect healing in amorphous Si3N4□Hy: An ab initio density functional theory study. *Physical Review B*, **2013**, 88,	3.3	13
11	NMR shieldings from density functional perturbation theory: GIPAW versus all-electron calculations. *Journal of Chemical Physics*, **2017**, 146, 064115	3.9	12
10	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	3.9	12
9	Nonlinear behavior of the band gap of Pb1□EuxSe (0□1) from first principles. *Physical Review B*, **2008**, 78,	3.3	9
8	OpenMP in VASP: Threading and SIMD. *International Journal of Quantum Chemistry*, **2019**, 119, e25851	2.1	8
7	Metastable surface oxide on CoGa(100): Structure and stability. *Physical Review B*, **2010**, 81,	3.3	7
6	Fast iterative interior eigensolver for millions of atoms. *Journal of Computational Physics*, **2012**, 231, 4836-4847	4.1	6
5	Formation of a Positive Fixed Charge at c□Si(111)/a□Si3N3.5:H Interfaces. *Physical Review Applied*, **2015**, 3,	4.3	5
4	Gaussian charge-transfer charge distributions for non-self-consistent electronic structure calculations. *Physical Review B*, **2012**, 85,	3.3	3
3	Electron-phonon interactions using the projector augmented-wave method and Wannier functions. *Physical Review B*, **2020**, 101,	3.3	2
2	Periodic Systems, Plane Waves, the PAW Method, and Hybrid Functionals61-76		
1	Comparing GIPAW with numerically exact chemical shieldings: The role of two-center contributions to the induced current.. *Journal of Chemical Physics*, **2021**, 155, 234101	3.9	