

# Martijn Marsman

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Comparing GIPAW with numerically exact chemical shieldings: The role of two-center contributions to the induced current.. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 234101	3.9	
34	Electron-phonon interactions using the projector augmented-wave method and Wannier functions. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	2
33	OpenMP in VASP: Threading and SIMD. <i>International Journal of Quantum Chemistry</i> , <b>2019</b> , 119, e25851	2.1	8
32	Charge self-consistent many-body corrections using optimized projected localized orbitals. <i>Journal of Physics Condensed Matter</i> , <b>2018</b> , 30, 475901	1.8	16
31	NMR shieldings from density functional perturbation theory: GIPAW versus all-electron calculations. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 064115	3.9	12
30	Embedding for bulk systems using localized atomic orbitals. <i>Journal of Chemical Physics</i> , <b>2017</b> , 147, 034130	3.0	16
29	Reproducibility in density functional theory calculations of solids. <i>Science</i> , <b>2016</b> , 351, aad3000	33.3	784
28	Iron as a source of efficient Shockley-Read-Hall recombination in GaN. <i>Applied Physics Letters</i> , <b>2016</b> , 109, 162107	3.4	50
27	Formation of a Positive Fixed Charge at cSi(111)/aBi3N3.5:H Interfaces. <i>Physical Review Applied</i> , <b>2015</b> , 3,	4.3	5
26	Anisotropic magnetic couplings and structure-driven canted to collinear transitions in Sr2IrO4 by magnetically constrained noncollinear DFT. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	55
25	Hyperfine coupling of point defects in semiconductors by hybrid density functional calculations: The role of core spin polarization. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	61
24	Finite-field implementation of NMR chemical shieldings for molecules: direct and converse gauge-including projector-augmented-wave methods. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 014109	3.9	12
23	Defects and defect healing in amorphous Si3N4:H: An ab initio density functional theory study. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	13
22	Fast iterative interior eigensolver for millions of atoms. <i>Journal of Computational Physics</i> , <b>2012</b> , 231, 4836-4847	4.1	6
21	Optical and electronic properties of Si3N4 and SiO2. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	50
20	Gaussian charge-transfer charge distributions for non-self-consistent electronic structure calculations. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	3
19	Density functional theory study of the structural and electronic properties of amorphous silicon nitrides: Si3N4:H. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	23

18	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 2780-5	6.4	95
17	Electric Control of Magnetization and Interplay between Orbital Ordering and Ferroelectricity in a Multiferroic Metal-Organic Framework. <i>Angewandte Chemie</i> , <b>2011</b> , 123, 5969-5972	3.6	50
16	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	138
15	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	59
14	Metastable surface oxide on CoGa(100): Structure and stability. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	7
13	Second-order Møller-Plesset perturbation theory applied to extended systems. II. Structural and energetic properties. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 074107	3.9	125
12	Making the random phase approximation to electronic correlation accurate. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 154115	3.9	199
11	Second-order Møller-Plesset perturbation theory applied to extended systems. I. Within the projector-augmented-wave formalism using a plane wave basis set. <i>Journal of Chemical Physics</i> , <b>2009</b> , 130, 184103	3.9	167
10	Hybrid functionals applied to extended systems. <i>Journal of Physics Condensed Matter</i> , <b>2008</b> , 20, 064201	1.8	430
9	Nonlinear behavior of the band gap of Pb <sub>1-x</sub> EuxSe (0 ≤ x ≤ 1) from first principles. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	9
8	Why does the B3LYP hybrid functional fail for metals?. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 024103	3.9	424
7	Accurate quasiparticle spectra from self-consistent GW calculations with vertex corrections. <i>Physical Review Letters</i> , <b>2007</b> , 99, 246403	7.4	529
6	Relaxed core projector-augmented-wave method. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 104101	3.9	93
5	Structural, electronic and magnetic properties of Gd investigated by DFT+U methods: bulk, clean and H-covered (0001) surfaces. <i>Journal of Physics Condensed Matter</i> , <b>2006</b> , 18, 7021-7043	1.8	51
4	Screened hybrid density functionals applied to solids. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 154709	3.9	1591
3	The Perdew-Burke-Ernzerhof exchange-correlation functional applied to the G2-1 test set using a plane-wave basis set. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 234102	3.9	560
2	Magnetic doping of 4d transition-metal surfaces: A first-principles study. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	19
1	Periodic Systems, Plane Waves, the PAW Method, and Hybrid Functionals 61-76		

