Martijn Marsman

List of Publications by Year in descending order

33 papers	7,363 citations	304368 22 h-index	377514 34 g-index
36 all docs	36 docs citations	36 times ranked	8625 citing authors

#	Article	IF	Citations
1	Comparing GIPAW with numerically exact chemical shieldings: the role of two-centre contributions to the induced current. Journal of Chemical Physics, 2021, 155, 234101.	1.2	0
2	Electron-phonon interactions using the projector augmented-wave method and Wannier functions. Physical Review B, 2020, 101, .	1.1	10
3	OpenMP in VASP: Threading and SIMD. International Journal of Quantum Chemistry, 2019, 119, e25851.	1.0	15
4	Charge self-consistent many-body corrections using optimized projected localized orbitals. Journal of Physics Condensed Matter, 2018, 30, 475901.	0.7	36
5	NMR shieldings from density functional perturbation theory: GIPAW versus all-electron calculations. Journal of Chemical Physics, 2017, 146, 064115.	1.2	15
6	Embedding for bulk systems using localized atomic orbitals. Journal of Chemical Physics, 2017, 147, 034110.	1.2	17
7	Iron as a source of efficient Shockley-Read-Hall recombination in GaN. Applied Physics Letters, 2016, 109, .	1.5	64
8	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
9	Formation of a Positive Fixed Charge at<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>c</mml:mi><mml:mtext>â</mml:mtext><mml:mi>Si</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 417.5 Td (stretchy="false" mathvariant="normal">N</mml:mi></mml:mrow><mml:mro. Physical Review Applied, 2015, 3, .	1.5	7
10	Anisotropic magnetic couplings and structure-driven canted to collinear transitions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>IrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi></mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> magnetically constrained noncollinear DFT. Physical Review B, 2015, 92, .	1.1	70
11	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
12	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
13	Defects and disorder in amorphous Si<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>: Density functional theory calculations. Physical Review B, 2013, 87, .	1.1	19
14	Optical and electronic properties of Si<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-SiO<mml:math xmlns:mml="http://www.w3.org/1998/	1.1	57
15	Gaussian charge-transfer charge distributions for non-self-consistent electronic structure calculations. Physical Review B, 2012, 85, .	1.1	3
16	Density functional theory study of the structural and electronic properties of amorphous silicon nitrides: Si<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>4</mml:mn><mml:mo>â</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>:H. Physical Review B, 2012, 86, .	1.1	34
17	Fast iterative interior eigensolver for millions of atoms. Journal of Computational Physics, 2012, 231, 4836-4847.	1.9	7
18	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. Physical Review B, 2011, 84, .	1.1	180

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19	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
20	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. Physical Review B, 2011, 83, .	1.1	67
21	Metastable surface oxide on CoGa(100): Structure and stability. Physical Review B, 2010, 81, .	1.1	7
22	Second-order MÃ¸llerâ€“Plesset perturbation theory applied to extended systems. II. Structural and energetic properties. Journal of Chemical Physics, 2010, 133, 074107.	1.2	147
23	Making the random phase approximation to electronic correlation accurate. Journal of Chemical Physics, 2009, 131, 154115.	1.2	227
24	Second-order MÃ¸llerâ€“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
25	Hybrid functionals applied to extended systems. Journal of Physics Condensed Matter, 2008, 20, 064201.	0.7	500
26	Nonlinear behavior of the band gap of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Pb</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> xmlns:mml="http://www.w3.org/1998/Math/MathML"		