Michiel Jan van Setten

List of Publications by Citations

51 papers	3,703 citations	24 h-index	53 g-index
53 ext. papers	4,642 ext. citations	5.6 avg, IF	5.19 L-index

#	Paper	IF	Citations
51	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
50	Recent developments in the ABINIT software package. *Computer Physics Communications*, **2016**, 205, 106-131	4.2	494
49	The PseudoDojo: Training and grading a 85 element optimized norm-conserving pseudopotential table. *Computer Physics Communications*, **2018**, 226, 39-54	4.2	473
48	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
47	The GW-Method for Quantum Chemistry Applications: Theory and Implementation. *Journal of Chemical Theory and Computation*, **2013**, 9, 232-46	6.4	174
46	Thermodynamic stability of boron: the role of defects and zero point motion. *Journal of the American Chemical Society*, **2007**, 129, 2458-65	16.4	147
45	The Abinitproject: Impact, environment and recent developments. *Computer Physics Communications*, **2020**, 248, 107042	4.2	143
44	Electronic structure and optical properties of lightweight metal hydrides. *Physical Review B*, **2007**, 75,	3.3	109
43	Quasi-Particle Self-Consistent GW for Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 2528-41	6.4	90
42	High-Throughput Design of Non-oxide p-Type Transparent Conducting Materials: Data Mining, Search Strategy, and Identification of Boron Phosphide. *Chemistry of Materials*, **2017**, 29, 2568-2573	9.6	79
41	High-throughput density-functional perturbation theory phonons for inorganic materials. *Scientific Data*, **2018**, 5, 180065	8.2	75
40	LiBH4Mg(BH4)2: A Physical Mixture of Metal Borohydrides as Hydrogen Storage Material. *Journal of Physical Chemistry C*, **2011**, 115, 6095-6101	3.8	73
39	A Density Functional Study of Mg(BH4)2. *Chemistry of Materials*, **2008**, 20, 4952-4956	9.6	70
38	Benchmark of GW Approaches for the GW100 Test Set. *Journal of Chemical Theory and Computation*, **2016**, 12, 5076-5087	6.4	63
37	GW100: A Plane Wave Perspective for Small Molecules. *Journal of Chemical Theory and Computation*, **2017**, 13, 635-648	6.4	58
36	Core-Level Binding Energies from GW: An Efficient Full-Frequency Approach within a Localized Basis. *Journal of Chemical Theory and Computation*, **2018**, 14, 4856-4869	6.4	55
35	Ab initio study of the effects of transition metal doping of Mg2NiH4. *Physical Review B*, **2007**, 76,	3.3	53

34	ABINIT: Overview and focus on selected capabilities. *Journal of Chemical Physics*, **2020**, 152, 124102	3.9	52
33	Ab initio study of Mg(AlH4)2. *Physical Review B*, **2005**, 72,	3.3	46
32	Assessing GW Approaches for Predicting Core Level Binding Energies. *Journal of Chemical Theory and Computation*, **2018**, 14, 877-883	6.4	37
31	Off-Diagonal Self-Energy Terms and Partially Self-Consistency in GW Calculations for Single Molecules: Efficient Implementation and Quantitative Effects on Ionization Potentials. *Journal of Chemical Theory and Computation*, **2015**, 11, 5152-60	6.4	36
30	Binding in alkali and alkaline-earth tetrahydroborates: Special position of magnesium tetrahydroborate. *Physical Review B*, **2010**, 81,	3.3	33
29	Automation methodologies and large-scale validation for GW: Towards high-throughput GW calculations. *Physical Review B*, **2017**, 96,	3.3	31
28	First-principles calculations of the crystal structure, electronic structure, and thermodynamic stability of Be(BH4)2. *Physical Review B*, **2008**, 77,	3.3	28
27	Hafnium-an optical hydrogen sensor spanning six orders in pressure. *Nature Communications*, **2017**, 8, 15718	17.4	23
26	A new phase in the decomposition of Mg(BH4)2: first-principles simulated annealing. *Journal of Materials Chemistry*, **2009**, 19, 7081		23
25	Hydrogenography of MgyNi1−xHx gradient thin films: Interplay between the thermodynamics and kinetics of hydrogenation. *Acta Materialia*, **2010**, 58, 658-668	8.4	23
24	Optical response of the sodium alanate system: GW0-BSE calculations and thin film measurements. *Physical Review B*, **2011**, 83,	3.3	19
23	First-principles investigation of the structural, dynamical, and dielectric properties of kesterite, stannite, and PMCA phases of Cu2ZnSnS4. *Physical Review B*, **2016**, 94,	3.3	18
22	HF Species and Dissolved Oxygen on the Epitaxial Lift-Off Process of GaAs Using AlAsP Release Layers. *Journal of the Electrochemical Society*, **2008**, 155, D35	3.9	16
21	Benchmarking the Fundamental Electronic Properties of small TiO Nanoclusters by GW and Coupled Cluster Theory Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3814-3828	6.4	15
20	Quantum size effects in the atomistic structure of armchair nanoribbons. *Physical Review B*, **2012**, 85,	3.3	15
19	First-principles study of the optical properties of MgxTi1−xH2. *Physical Review B*, **2009**, 79,	3.3	15
18	Reproducibility in G0W0 calculations for solids. *Computer Physics Communications*, **2020**, 255, 107242	4.2	14
17	On the enthalpy of formation of aluminum diboride, AlB2. *Journal of Alloys and Compounds*, **2009**, 477, L11-L12	5.7	13

16	Insights into cation disorder and phase transitions in CZTS from a first-principles approach. *Physical Review Materials*, **2018**, 2,	3.2	12
15	First-principles study of paraelectric and ferroelectric CsH2PO4 including dispersion forces: Stability and related vibrational, dielectric, and elastic properties. *Physical Review B*, **2017**, 95,	3.3	11
14	Computationally driven high-throughput identification of CaTe and Li3Sb as promising candidates for high-mobility p-type transparent conducting materials. *Physical Review Materials*, **2019**, 3,	3.2	11
13	First-principles modelling of magnesium titanium hydrides. *Journal of Physics Condensed Matter*, **2010**, 22, 074208	1.8	10
12	Lightweight sodium alanate thin films grown by reactive sputtering. *Applied Physics Letters*, **2009**, 95, 121904	3.4	10
11	In-Situ Deposition of Alkali and Alkaline Earth Hydride Thin Films To Investigate the Formation of Reactive Hydride Composites. *Journal of Physical Chemistry C*, **2010**, 114, 13895-13901	3.8	9
10	Model for the Formation Energies of Alanates and Boranates. *Journal of Physical Chemistry C*, **2007**, 111, 9592-9594	3.8	9
9	The GW Miracle in Many-Body Perturbation Theory for the Ionization Potential of Molecules.. *Frontiers in Chemistry*, **2021**, 9, 749779	5	7
8	Incommensurate Quantum Size Oscillations of Oligoacene Wires Adsorbed on Au(111). *Journal of Physical Chemistry C*, **2019**, 123, 8902-8907	3.8	6
7	(Invited) Sub-40mV Sigma VTH Igzo nFETs in 300mm Fab. *ECS Transactions*, **2020**, 98, 205-217	1	4
6	Oxygen Defect Stability in Amorphous, C-Axis Aligned, and Spinel IGZO. *ACS Applied Electronic Materials*, **2021**, 3, 4037-4046	4	4
5	Polarization-dependent Raman spectroscopy of LiBH4 single crystals and Mg(BH4)2 powders. *Journal of Raman Spectroscopy*, **2011**, 42, 1796-1801	2.3	3
4	Deposition, Characterization, and Performance of Spinel InGaZnO4. *ACS Applied Electronic Materials* , **2022**, 4, 1238-1249	4	2
3	Electronic Structure and Formation Enthalpy of Hydroaluminates and Hydroborates **2008**, 1-6		1
2	A First-Principles Tool to Discover New Pyrometallurgical Refining Options. *Jom*, **2021**, 73, 2900-2910	2.1	0
1	On the elastic tensors of ultra-thin films: A study of ruthenium. *Applied Surface Science*, **2022**, 153194	6.7	0