Michiel Jan van Setten

List of Publications by Year in Descending Order

Source: https://exaly.com/author-pdf/7447749/michiel-jan-van-setten-publications-by-year.pdf
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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	Deposition, Characterization, and Performance of Spinel InGaZnO4. *ACS Applied Electronic Materials* , **2022**, 4, 1238-1249	4	2
50	On the elastic tensors of ultra-thin films: A study of ruthenium. *Applied Surface Science*, **2022**, 153194	6.7	0
49	A First-Principles Tool to Discover New Pyrometallurgical Refining Options. *Jom*, **2021**, 73, 2900-2910	2.1	0
48	Oxygen Defect Stability in Amorphous, C-Axis Aligned, and Spinel IGZO. *ACS Applied Electronic Materials*, **2021**, 3, 4037-4046	4	4
47	The GW Miracle in Many-Body Perturbation Theory for the Ionization Potential of Molecules.. *Frontiers in Chemistry*, **2021**, 9, 749779	5	7
46	Reproducibility in G0W0 calculations for solids. *Computer Physics Communications*, **2020**, 255, 107242	4.2	14
45	ABINIT: Overview and focus on selected capabilities. *Journal of Chemical Physics*, **2020**, 152, 124102	3.9	52
44	(Invited) Sub-40mV Sigma VTH Igzo nFETs in 300mm Fab. *ECS Transactions*, **2020**, 98, 205-217	1	4
43	The Abinitproject: Impact, environment and recent developments. *Computer Physics Communications*, **2020**, 248, 107042	4.2	143
42	Incommensurate Quantum Size Oscillations of Oligoacene Wires Adsorbed on Au(111). *Journal of Physical Chemistry C*, **2019**, 123, 8902-8907	3.8	6
41	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
40	The PseudoDojo: Training and grading a 85 element optimized norm-conserving pseudopotential table. *Computer Physics Communications*, **2018**, 226, 39-54	4.2	473
39	Assessing GW Approaches for Predicting Core Level Binding Energies. *Journal of Chemical Theory and Computation*, **2018**, 14, 877-883	6.4	37
38	High-throughput density-functional perturbation theory phonons for inorganic materials. *Scientific Data*, **2018**, 5, 180065	8.2	75
37	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
36	Insights into cation disorder and phase transitions in CZTS from a first-principles approach. *Physical Review Materials*, **2018**, 2,	3.2	12
35	GW100: A Plane Wave Perspective for Small Molecules. *Journal of Chemical Theory and Computation* , **2017**, 13, 635-648	6.4	58

34	First-principles study of paraelectric and ferroelectric CsH_2PO_4 including dispersion forces: Stability and related vibrational, dielectric, and elastic properties. *Physical Review B*, **2017**, 95,	3.3	11
33	Hafnium-an optical hydrogen sensor spanning six orders in pressure. *Nature Communications*, **2017**, 8, 15718	17.4	23
32	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
31	Automation methodologies and large-scale validation for GW: Towards high-throughput GW calculations. *Physical Review B*, **2017**, 96,	3.3	31
30	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
29	Benchmark of GW Approaches for the GW100 Test Set. *Journal of Chemical Theory and Computation*, **2016**, 12, 5076-5087	6.4	63
28	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
27	First-principles investigation of the structural, dynamical, and dielectric properties of kesterite, stannite, and PMCA phases of Cu_2ZnSnS_4. *Physical Review B*, **2016**, 94,	3.3	18
26	Recent developments in the ABINIT software package. *Computer Physics Communications*, **2016**, 205, 106-131	4.2	494
25	Quasi-Particle Self-Consistent GW for Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 2528-41	6.4	90
24	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
23	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
22	The GW-Method for Quantum Chemistry Applications: Theory and Implementation. *Journal of Chemical Theory and Computation*, **2013**, 9, 232-46	6.4	174
21	Quantum size effects in the atomistic structure of armchair nanoribbons. *Physical Review B*, **2012**, 85,	3.3	15
20	Polarization-dependent Raman spectroscopy of $LiBH_4$ single crystals and $Mg(BH_4)_2$ powders. *Journal of Raman Spectroscopy*, **2011**, 42, 1796-1801	2.3	3
19	$LiBH_4$Mg$(BH_4)_2$: A Physical Mixture of Metal Borohydrides as Hydrogen Storage Material. *Journal of Physical Chemistry C*, **2011**, 115, 6095-6101	3.8	73
18	Optical response of the sodium alanate system: GW0-BSE calculations and thin film measurements. *Physical Review B*, **2011**, 83,	3.3	19
17	First-principles modelling of magnesium titanium hydrides. *Journal of Physics Condensed Matter*, **2010**, 22, 074208	1.8	10

16	Binding in alkali and alkaline-earth tetrahydroborates: Special position of magnesium tetrahydroborate. *Physical Review B*, **2010**, 81,	3.3	33
15	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
14	Hydrogenography of MgyNi1yHx gradient thin films: Interplay between the thermodynamics and kinetics of hydrogenation. *Acta Materialia*, **2010**, 58, 658-668	8.4	23
13	First-principles study of the optical properties of MgxTi1xH2. *Physical Review B*, **2009**, 79,	3.3	15
12	On the enthalpy of formation of aluminum diboride, AlB2. *Journal of Alloys and Compounds*, **2009**, 477, L11-L12	5.7	13
11	A new phase in the decomposition of Mg(BH4)2: first-principles simulated annealing. *Journal of Materials Chemistry*, **2009**, 19, 7081		23
10	Lightweight sodium alanate thin films grown by reactive sputtering. *Applied Physics Letters*, **2009**, 95, 121904	3.4	10
9	First-principles calculations of the crystal structure, electronic structure, and thermodynamic stability of Be(BH4)2. *Physical Review B*, **2008**, 77,	3.3	28
8	A Density Functional Study of Mg(BH4)2. *Chemistry of Materials*, **2008**, 20, 4952-4956	9.6	70
7	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
6	Electronic Structure and Formation Enthalpy of Hydroaluminates and Hydroborates **2008**, 1-6		1
5	Model for the Formation Energies of Alanates and Boranates. *Journal of Physical Chemistry C*, **2007**, 111, 9592-9594	3.8	9
4	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
3	Electronic structure and optical properties of lightweight metal hydrides. *Physical Review B*, **2007**, 75,	3.3	109
2	Ab initio study of the effects of transition metal doping of Mg2NiH4. *Physical Review B*, **2007**, 76,	3.3	53
1	Ab initio study of Mg(AlH4)2. *Physical Review B*, **2005**, 72,	3.3	46