Gilles A De Wijs

List of Publications by Citations

109 papers	4,512 citations	37 h-index	64 g-index
117 ext. papers	4,894 ext. citations	4.8 avg, IF	5.28 L-index

#	Paper	IF	Citations
109	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
108	The viscosity of liquid iron at the physical conditions of the Earth's core. *Nature*, **1998**, 392, 805-807	50.4	232
107	Modeling the polymorphism of pentacene. *Journal of the American Chemical Society*, **2003**, 125, 6323-30	16.4	198
106	Mixed Magnetism for Refrigeration and Energy Conversion. *Advanced Energy Materials*, **2011**, 1, 1215-1219	12.8	192
105	Spin-polarization in half-metals (invited). *Journal of Applied Physics*, **2002**, 91, 8340	2.5	173
104	Towards 100% spin-polarized charge-injection: The half-metallic NiMnSb/CdS interface. *Physical Review B*, **2001**, 64,	3.3	166
103	The electronic structure of tantalum (oxy)nitridesTaON and Ta3N5. *Journal of Materials Chemistry*, **2001**, 11, 1248-1252		164
102	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
101	Anisotropy of the mobility of pentacene from frustration. *Synthetic Metals*, **2003**, 139, 109-114	3.6	123
100	First-order phase transitions by first-principles free-energy calculations: The melting of Al. *Physical Review B*, **1998**, 57, 8223-8234	3.3	115
99	Electronic structure and optical properties of lightweight metal hydrides. *Physical Review B*, **2007**, 75,	3.3	109
98	DFT Study of Planar Boron Sheets: A New Template for Hydrogen Storage. *Journal of Physical Chemistry C*, **2009**, 113, 18962-18967	3.8	101
97	Modeling and analysis of the three-dimensional current density in sandwich-type single-carrier devices of disordered organic semiconductors. *Physical Review B*, **2009**, 79,	3.3	98
96	First principles calculations on crystalline and liquid iron at Earth's core conditions. *Faraday Discussions*, **1997**, 106, 205-218	3.6	94
95	Structure and electronic properties of amorphous WO3. *Physical Review B*, **1999**, 60, 16463-16474	3.3	79
94	A Density Functional Study of □Mg(BH4)2. *Chemistry of Materials*, **2008**, 20, 4952-4956	9.6	70
93	Ab initio and work function and surface energy anisotropy of LaB6. *Journal of Physical Chemistry B*, **2006**, 110, 18459-65	3.4	69

92	Role of Magnetism in Catalysis: RuO2 (110) Surface. *Journal of Physical Chemistry C*, **2013**, 117, 6353-6357	3.8	64
91	Symmetry, Dynamics, and Defects in Methylammonium Lead Halide Perovskites. *Journal of Physical Chemistry Letters*, **2017**, 8, 61-66	6.4	63
90	The Role of Connectivity on Electronic Properties of Lead Iodide Perovskite-Derived Compounds. *Inorganic Chemistry*, **2017**, 56, 8408-8414	5.1	59
89	Local structure and electronic properties of BaTaO2N with perovskite-type structure. *Journal of Physics and Chemistry of Solids*, **2003**, 64, 281-286	3.9	59
88	Anionogenic ferromagnets. *Journal of the American Chemical Society*, **2005**, 127, 16325-8	16.4	58
87	Li intercalation in graphite: A van der Waals density-functional study. *Physical Review B*, **2014**, 90,	3.3	56
86	First-principles calculation of the phonon spectrum of MgAl2O4 spinel. *Physical Review B*, **2002**, 65,	3.3	56
85	Ab initio study of the effects of transition metal doping of Mg2NiH4. *Physical Review B*, **2007**, 76,	3.3	53
84	First-principles study of hydrogenated amorphous silicon. *Physical Review B*, **2009**, 79,	3.3	49
83	Mechanism for SiCl2 Formation and Desorption and the Growth of Pits in the Etching of Si(100) with Chlorine. *Physical Review Letters*, **1997**, 78, 4877-4880	7.4	49
82	Phonon spectrum of ZnAl2O4 spinel from inelastic neutron scattering and first-principles calculations. *Physical Review B*, **2002**, 66,	3.3	49
81	Ab initio study of Mg(AlH4)2. *Physical Review B*, **2005**, 72,	3.3	46
80	Amorphous WO3: a first-principles approach. *Electrochimica Acta*, **2001**, 46, 1989-1993	6.7	46
79	Tunable hydrogen storage in magnesium transition metal compounds: First-principles calculations. *Physical Review B*, **2009**, 79,	3.3	45
78	Phonon spectrum and thermal properties of cubic Si3N4 from first-principles calculations. *Journal of Applied Physics*, **2003**, 93, 5175-5180	2.5	44
77	First-principles study of chlorine adsorption and reactions on Si(100). *Physical Review B*, **1998**, 57, 10021-10029	3.3	44
76	Electronic band structure of tetracene-TCNQ and perylene-TCNQ compounds. *Journal of Physical Chemistry A*, **2008**, 112, 2497-502	2.8	41
75	The continuing drama of the half-metal/semiconductor interface. *Journal Physics D: Applied Physics*, **2006**, 39, 793-796	3	39

74	Tunable spin transport in CrAs: Role of correlation effects. *Physical Review B*, **2005**, 71,	3.3	38
73	Hydrogen Storage by Polylithiated Molecules and Nanostructures. *Journal of Physical Chemistry C*, **2009**, 113, 8997-9002	3.8	37
72	First-principles molecular-dynamics simulation of liquid CsPb. *Journal of Chemical Physics*, **1995**, 103, 5031-5040	3.9	36
71	Crystal Growth, Structure, and Electronic Band Structure of Tetracene TCNQ. *Journal of Physical Chemistry C*, **2007**, 111, 3486-3489	3.8	34
70	The electronic structure of organic-inorganic hybrid compounds: (NH)CuCl, (CHNNH)CuCl and (CHNNH)CuCl. *Journal of Physics Condensed Matter*, **2013**, 25, 295502	1.8	33
69	Defects in half-metals and finite temperature. *Journal of Physics Condensed Matter*, **2004**, 16, S5517-S5524	1.8	33
68	Phonons and electron-phonon coupling in graphene-h-BN heterostructures. *Annalen Der Physik*, **2014**, 526, 381-386	2.6	31
67	Electron-ion correlation in liquid metals from first principles: Liquid Mg and liquid Bi. *Physical Review Letters*, **1995**, 75, 4480-4483	7.4	31
66	Geometry of {001} Surfaces of Spinel (MgAl2O4): First-Principles Simulations and Experimental Measurements. *Journal of the American Ceramic Society*, **2005**, 88, 1544-1548	3.8	30
65	First-principles calculations of the crystal structure, electronic structure, and thermodynamic stability of Be(BH4)2. *Physical Review B*, **2008**, 77,	3.3	28
64	Spin tunneling in junctions with disordered ferromagnets. *Physical Review Letters*, **2008**, 100, 057205	7.4	28
63	O/N Ordering in Y2Si3O3N4 with the Melilite-type Structure from First-Principles Calculations. *Chemistry of Materials*, **2000**, 12, 1071-1075	9.6	27
62	A solid-state NMR and DFT study of compositional modulations in Al(x)Ga(1-x)As. *Physical Chemistry Chemical Physics*, **2010**, 12, 11517-35	3.6	25
61	Bond Scission in a Perfect Polyethylene Chain and the Consequences for the Ultimate Strength. *Macromolecules*, **2000**, 33, 9098-9108	5.5	25
60	Hydrogen bonding and chemical shift assignments in carbazole functionalized isocyanides from solid-state NMR and first-principles calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 13082-95	3.6	24
59	Improved hydrogen storage in Ca-decorated boron heterofullerenes: a theoretical study. *Journal of Materials Chemistry A*, **2015**, 3, 7710-7714	13	23
58	Interactions of adsorbed CO on water ice at low temperatures. *Physical Chemistry Chemical Physics*, **2014**, 16, 15630-9	3.6	22
57	Patterning of Si(001) with halogens: Surface structure as a function of the halogen chemical potential. *Physical Review B*, **2001**, 64,	3.3	22

56	Bulk and Surface Electronic Structure of the Layered Sub-Nitrides Ca2N and Sr2N. *Chemistry of Materials*, **2000**, 12, 1847-1852	9.6	22
55	First-Principles Study of LiBH4 Nanoclusters and Their Hydrogen Storage Properties. *Journal of Physical Chemistry C*, **2012**, 116, 18038-18047	3.8	21
54	k□p subband structure of the LaAlO3/SrTiO3 interface. *Physical Review B*, **2013**, 88,	3.3	21
53	Spintronic materials based on main-group elements. *Journal of Physics Condensed Matter*, **2007**, 19, 165208	1.8	21
52	Chlorine on Si(001)-(2 x 1): Bridge versus Terminal Bonding. *Physical Review Letters*, **1996**, 77, 881-884	7.4	21
51	First-principles molecular-dynamics simulation of liquid Li12Si7. *Physical Review B*, **1993**, 48, 13459-13468	3.3	21
50	Tuning the Hydrogen Storage in Magnesium Alloys. *Journal of Physical Chemistry Letters*, **2010**, 1, 1982-1986	6.4	20
49	Atomistic models of hydrogenated amorphous silicon nitride from first principles. *Physical Review B* , **2010**, 82,	3.3	20
48	Optical response of the sodium alanate system: GW0-BSE calculations and thin film measurements. *Physical Review B*, **2011**, 83,	3.3	19
47	Optimizing performance of half-metals at finite temperature. *Journal of Physics Condensed Matter*, **2007**, 19, 315212	1.8	18
46	The role of the hydrogen bonding network for the shear modulus of PIPD. *Polymer*, **2005**, 46, 9144-9154	3.9	18
45	Geometric, electronic, and magnetic structure of FexOy+ clusters. *Physical Review B*, **2015**, 92,	3.3	17
44	Work function anisotropy and surface stability of half-metallic CrO2. *Physical Review B*, **2008**, 77,	3.3	17
43	Local Structure and Chemical Bonding of Protonated LixMn2O4 Spinels from First Principles. *Chemistry of Materials*, **2006**, 18, 1169-1173	9.6	17
42	Low work function of the (1000) Ca2N surface. *Journal of Applied Physics*, **2004**, 96, 1751-1753	2.5	17
41	First-principles study of the optical properties of MgxTi1□H2. *Physical Review B*, **2009**, 79,	3.3	15
40	Intrinsic defects and dopants in LiNH2: a first-principles study. *Physical Chemistry Chemical Physics*, **2011**, 13, 6043-52	3.6	14
39	Theoretical study of the stable radicals galvinoxyl, azagalvinoxyl and wurster's blue perchlorate in the solid state. *Journal of Physical Chemistry A*, **2008**, 112, 7734-8	2.8	14

38	Lattice and local-mode vibrations in anhydrous and protonized LiMn2O4 spinels from first-principles theory. *Journal of Materials Chemistry*, **2007**, 17, 4908		14
37	Microscopic (Dis)order and Dynamics of Cations in Mixed FA/MA Lead Halide Perovskites. *Journal of Physical Chemistry C*, **2021**, 125, 1742-1753	3.8	14
36	Reversed spin polarization at the Co(001)-HfO2(001) interface. *Physical Review B*, **1998**, 58, 15422-15425	3.3	13
35	Nanometre superstructure in liquid alkali-thallium alloys. *Journal of Physics Condensed Matter*, **1993**, 5, 9253-9260	1.8	13
34	NMR shieldings from density functional perturbation theory: GIPAW versus all-electron calculations. *Journal of Chemical Physics*, **2017**, 146, 064115	3.9	12
33	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
32	Native Defects and the Dehydrogenation of NaBH4. *Journal of Physical Chemistry C*, **2011**, 115, 24429-24434	3.8	12
31	Clusters in liquid K-Tl and Cs-Tl alloys. *Journal of Physics Condensed Matter*, **1994**, 6, A255-A260	1.8	12
30	Carbon Support Effects on the Hydrogen Storage Properties of LiBH4 Nanoparticles: A First-Principles Study. *Journal of Physical Chemistry C*, **2014**, 118, 5102-5109	3.8	11
29	Transport coefficients of liquids from first principles. *Journal of Non-Crystalline Solids*, **1999**, 250-252, 82-90	3.9	11
28	First-principles modelling of magnesium titanium hydrides. *Journal of Physics Condensed Matter*, **2010**, 22, 074208	1.8	10
27	Switchable Fermi surface sheets in greigite. *Physical Review B*, **2012**, 86,	3.3	10
26	Model for the Formation Energies of Alanates and Boranates. *Journal of Physical Chemistry C*, **2007**, 111, 9592-9594	3.8	9
25	Interrelation of Work Function and Surface Stability: The Case of BaAl4. *Chemistry of Materials*, **2005**, 17, 3879-3882	9.6	9
24	Structural Studies of Polyaramid Fibers: Solid-State NMR and First-Principles Modeling. *Macromolecules*, **2016**, 49, 5548-5560	5.5	9
23	Excess manganese as the origin of the low-temperature anomaly in NiMnSb. *Physical Review B*, **2013**, 88,	3.3	8
22	Generalised coexistence of a low work function and a stable surface: CaAl4 and BaAuIn3. *Surface Science*, **2006**, 600, 2495-2500	1.8	7
21	Structure of liquid caesium-lead alloys. *Journal of Non-Crystalline Solids*, **1993**, 156-158, 34-37	3.9	7

20	Band Offsets at the Interface between Crystalline and Amorphous Silicon from First Principles. *Physical Review Applied*, **2017**, 8,	4.3	7
19	The Rich Solid-State Phase Behavior of dl-Aminoheptanoic Acid: Five Polymorphic Forms and Their Phase Transitions. *Crystal Growth and Design*, **2018**, 18, 242-252	3.5	7
18	Preactive Site in ZieglerNatta Catalysts. *Journal of Physical Chemistry C*, **2019**, 123, 14490-14500	3.8	6
17	Theoretical models of Rashba spin splitting in asymmetric SrTiO3-based heterostructures. *Physical Review B*, **2017**, 95,	3.3	6
16	Lattice vibrations and thermal properties of carbon nitride with defect ZnS structure from first-principles calculations. *Journal of Physics Condensed Matter*, **2004**, 16, 3027-3034	1.8	6
15	Lithium trapping by excess oxygen in WO3: A first-principles study. *Physical Review B*, **2000**, 62, 1508-1513	3.3	6
14	q-GRID: A New Method To Calculate Lattice and Interaction Energies for Molecular Crystals from Electron Densities. *Crystal Growth and Design*, **2016**, 16, 662-671	3.5	5
13	Stripline 75As NMR Study of Epitaxial III–V Semiconductor Al0.5Ga0.5As. *Journal of Physical Chemistry C*, **2014**, 118, 13394-13405	3.8	4
12	Quantum confinement and band offsets in amorphous silicon quantum wells. *Physical Review B*, **2014**, 90,	3.3	4
11	Publisher's Note: Modeling and analysis of the three-dimensional current density in sandwich-type single-carrier devices of disordered organic semiconductors [Phys. Rev. B 79, 085203 (2009)]. *Physical Review B*, **2009**, 79,	3.3	4
10	Anionogenic mixed valency in KxBa1-xO2-. *Inorganic Chemistry*, **2014**, 53, 496-502	5.1	3
9	First-Principles Study of Structural Prototypes for NaAlH4: Elevated Pressure Polymorph in Symmetry Fmm2 Leads to a Single-Step Decomposition Pathway. *Journal of Physical Chemistry C*, **2013**, 117, 8864-8870	3.8	3
8	Weakening of a Polyethylene Chain by Methyl Side Groups. *Soft Materials*, **2003**, 1, 223-233	1.7	3
7	Structural models of a-Si:H with a low defect concentration: A first-principles molecular dynamics study. *Physica Status Solidi (A) Applications and Materials Science*, **2010**, 207, 605-608	1.6	2
6	A multi-nuclear magnetic resonance and density functional theory investigation of epitaxially grown InGaP2. *Physical Chemistry Chemical Physics*, **2016**, 18, 21296-304	3.6	2
5	Amorphous semiconductors studied by first-principles simulations: structure and electronic properties. *Materials Research Society Symposia Proceedings*, **2009**, 1153, 1		1
4	Ab initio molecular dynamics study of liquid Li12Si7. *Journal of Non-Crystalline Solids*, **1993**, 156-158, 961-964	3.9	1
3	Impact of F and S doping on (Mn,Fe)2(P,Si) giant magnetocaloric materials. *Acta Materialia*, **2022**, 234, 118057	8.4	1

2 Quantum mechanics calculations on the diastereomeric salts of cyclic phosphoric acids with ephedrine. *Computational and Theoretical Chemistry*, **2005**, 717, 205-214

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