Gilles A De Wijs

List of Publications by Year
in descending order

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111 papers	5,226 citations	81743 39 h-index	88477 70 g-index
117 all docs	117 docs citations	117 times ranked	6704 citing authors

#	Article	IF	Citations
1	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
2	The viscosity of liquid iron at the physical conditions of the Earth's core. Nature, 1998, 392, 805-807.	13.7	259
3	Mixed Magnetism for Refrigeration and Energy Conversion. Advanced Energy Materials, 2011, 1, 1215-1219.	10.2	227
4	Modeling the Polymorphism of Pentacene. Journal of the American Chemical Society, 2003, 125, 6323-6330.	6.6	214
5	Spin-polarization in half-metals (invited). Journal of Applied Physics, 2002, 91, 8340.	1.1	201
6	Towards 100% spin-polarized charge-injection: The half-metallic NiMnSb/CdS interface. Physical Review B, 2001, 64, .	1.1	184
7	The electronic structure of tantalum (oxy)nitrides TaON and Ta3N5. Journal of Materials Chemistry, 2001, 11, 1248-1252.	6.7	178
8	Thermodynamic Stability of Boron:Â The Role of Defects and Zero Point Motion. Journal of the American Chemical Society, 2007, 129, 2458-2465.	6.6	169
9	DFT Study of Planar Boron Sheets: A New Template for Hydrogen Storage. Journal of Physical Chemistry C, 2009, 113, 18962-18967.	1.5	130
10	Anisotropy of the mobility of pentacene from frustration. Synthetic Metals, 2003, 139, 109-114.	2.1	125
11	First-order phase transitions by first-principles free-energy calculations: The melting of Al. Physical Review B, 1998, 57, 8223-8234.	1.1	124
12	Electronic structure and optical properties of lightweight metal hydrides. Physical Review B, 2007, 75, .	1.1	120
13	First principles calculations on crystalline and liquid iron at Earth's core conditions. Faraday Discussions, 1997, 106, 205-218.	1.6	106
14	Modeling and analysis of the three-dimensional current density in sandwich-type single-carrier devices of disordered organic semiconductors. Physical Review B, 2009, 79, .	1.1	105
15	Role of Magnetism in Catalysis: RuO₂ (110) Surface. Journal of Physical Chemistry C, 2013, 117, 6353-6357.	1.5	98
16	Structure and electronic properties of amorphousWO3. Physical Review B, 1999, 60, 16463-16474.	1.1	88
17	The Role of Connectivity on Electronic Properties of Lead Iodide Perovskite-Derived Compounds. Inorganic Chemistry, 2017, 56, 8408-8414.	1.9	83
18	A Density Functional Study of Î±-Mg(BH4)2. Chemistry of Materials, 2008, 20, 4952-4956.	3.2	76

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19	Symmetry, Dynamics, and Defects in Methylammonium Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2017, 8, 61-66.	2.1	75
20	Ab Initio and Work Function and Surface Energy Anisotropy of LaB6. Journal of Physical Chemistry B, 2006, 110, 18459-18465.	1.2	74
21	Local structure and electronic properties of BaTaO2N with perovskite-type structure. Journal of Physics and Chemistry of Solids, 2003, 64, 281-286.	1.9	67
22	First-principles calculation of the phonon spectrum ofMgAl2O4spinel. Physical Review B, 2002, 65, .	1.1	66
23	Li intercalation in graphite: A van der Waals density-functional study. Physical Review B, 2014, 90, .	1.1	63
24	Anionogenic Ferromagnets. Journal of the American Chemical Society, 2005, 127, 16325-16328.	6.6	62
25	Ab initio study of the effects of transition metal doping of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Mg</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Ni</mml:mi><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2007, 76, .	1.1	61
26	First-principles study of hydrogenated amorphous silicon. Physical Review B, 2009, 79, .	1.1	61
27	Phonon spectrum ofZnAl2O4spinel from inelastic neutron scattering and first-principles calculations. Physical Review B, 2002, 66, .	1.1	60
28	Mechanism for SiCl2Formation and Desorption and the Growth of Pits in the Etching of Si(100) with Chlorine. Physical Review Letters, 1997, 78, 4877-4880.	2.9	54
29	Amorphous WO3: a first-principles approach. Electrochimica Acta, 2001, 46, 1989-1993.	2.6	52
30	First-principles study of chlorine adsorption and reactions onSi(100). Physical Review B, 1998, 57, 10021-10029.	1.1	50
31	Phonon spectrum and thermal properties of cubic Si3N4 from first-principles calculations. Journal of Applied Physics, 2003, 93, 5175-5180.	1.1	50
32	Ab initiostudy ofMg(AlH4)2. Physical Review B, 2005, 72, .	1.1	49
33	Tunable hydrogen storage in magnesiumâ€“transition metal compounds: First-principles calculations. Physical Review B, 2009, 79, .	1.1	48
34	Electronic Band Structure of Tetraceneâ^'TCNQ and Peryleneâ^'TCNQ Compounds. Journal of Physical Chemistry A, 2008, 112, 2497-2502.	1.1	46
35	The continuing drama of the half-metal/semiconductor interface. Journal Physics D: Applied Physics, 2006, 39, 793-796.	1.3	45
36	Tunable spin transport in CrAs: Role of correlation effects. Physical Review B, 2005, 71, .	1.1	40

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37	Phonons and electronâ€phonon coupling in grapheneâ€hâ€BN heterostructures. Annalen Der Physik, 2014, 526, 381-386.	0.9	40
38	Hydrogen Storage by Polylithiated Molecules and Nanostructures. Journal of Physical Chemistry C, 2009, 113, 8997-9002.	1.5	39
39	The electronic structure of organicâ€ inorganic hybrid compounds: (NH₄)₂CuCl₄, (CH₃NH₃)₂CuCl₄and (C₂H₅NH₃)₂CuCl₄. Journal of Physics Condensed Matter, 2013, 25, 205502.	0.7	39
40	Firstâ€principles molecularâ€dynamics simulation of liquid CsPb. Journal of Chemical Physics, 1995, 103, 5031-5040.	1.2	38
41	Crystal Growth, Structure, and Electronic Band Structure of Tetraceneâ^'TCNQ. Journal of Physical Chemistry C, 2007, 111, 3486-3489.	1.5	38
42	Defects in half-metals and finite temperature. Journal of Physics Condensed Matter, 2004, 16, S5517-S5524.	0.7	37
43	Electron-Ion Correlation in Liquid Metals from First Principles: Liquid Mg and Liquid Bi. Physical Review Letters, 1995, 75, 4480-4483.	2.9	36
44	Geometry of {001} Surfaces of Spinel (MgAl2O4): First-Principles Simulations and Experimental Measurements. Journal of the American Ceramic Society, 2005, 88, 1544-1548.	1.9	34
45	Bond Scission in a Perfect Polyethylene Chain and the Consequences for the Ultimate Strength. Macromolecules, 2000, 33, 9098-9108.	2.2	32
46	First-principles calculations of the crystal structure, electronic structure, and thermodynamic stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Be</mml:mtext><mml:msub><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow> Physical Review B, 2008, 77, .	1.1	31
47	Spin Tunneling in Junctions with Disordered Ferromagnets. Physical Review Letters, 2008, 100, 057205.	2.9	31
48	A solid-state NMR and DFT study of compositional modulations in AlxGa1â^'xAs. Physical Chemistry Chemical Physics, 2010, 12, 11517.	1.3	29
49	Bulk and Surface Electronic Structure of the Layered Sub-Nitrides Ca2N and Sr2N. Chemistry of Materials, 2000, 12, 1847-1852.	3.2	28
50	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.	1.3	28
51	Improved hydrogen storage in Ca-decorated boron heterofullerenes: a theoretical study. Journal of Materials Chemistry A, 2015, 3, 7710-7714.	5.2	28
52	Microscopic (Dis)order and Dynamics of Cations in Mixed FA/MA Lead Halide Perovskites. Journal of Physical Chemistry C, 2021, 125, 1742-1753.	1.5	28
53	O/N Ordering in Y2Si3O3N4 with the Melilite-type Structure from First-Principles Calculations. Chemistry of Materials, 2000, 12, 1071-1075.	3.2	27
54	Spintronic materials based on main-group elements. Journal of Physics Condensed Matter, 2007, 19, 165203.	0.7	26

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55	Tuning the Hydrogen Storage in Magnesium Alloys. Journal of Physical Chemistry Letters, 2010, 1, 1982-1986.	2.1	25
56	k<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>Â·</mml:mo></mml:math>p subband structure of the LaAlO<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>/SrTiO<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>interface. Physical Review B, 2013, 88, .	1.1	25
57	Interactions of adsorbed CO2 on water ice at low temperatures. Physical Chemistry Chemical Physics, 2014, 16, 15630.	1.3	25
58	Patterning of Si(001) with halogens: Surface structure as a function of the halogen chemical potential. Physical Review B, 2001, 64, .	1.1	23
59	First-Principles Study of LiBH4Nanoclusters and Their Hydrogen Storage Properties. Journal of Physical Chemistry C, 2012, 116, 18038-18047.	1.5	23
60	Chlorine onSi(001)â˜(2Ã—1): Bridge versus Terminal Bonding. Physical Review Letters, 1996, 77, 881-884.	2.9	22
61	Atomistic models of hydrogenated amorphous silicon nitride from first principles. Physical Review B, 2010, 82, .	1.1	22
62	First-principles molecular-dynamics simulation of liquidLi12Si7. Physical Review B, 1993, 48, 13459-13468.	1.1	21
63	Low work function of the (1000) Ca2N surface. Journal of Applied Physics, 2004, 96, 1751-1753.	1.1	21
64	Local Structure and Chemical Bonding of Protonated LixMn2O4Spinels from First Principles. Chemistry of Materials, 2006, 18, 1169-1173.	3.2	20
65	Optimizing performance of half-metals at finite temperature. Journal of Physics Condensed Matter, 2007, 19, 315212.	0.7	20
66	First-principles study of the optical properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mg</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub> Physical Review B, 2009, 79, .	1.1	20
67	Optical response of the sodium alanate system:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="italic">GW</mml:mi><mml:mrow><mml:mn>0</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>-BSE calculations and thin film measurements. Physical Review B, 2011, 83, .	1.1	20
68	Geometric, electronic, and magnetic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mtext>Fe</mml:mtext><mml:mi>x</mml:mi></ Physical Review B, 2015, 92, .	1.1	19
69	The role of the hydrogen bonding network for the shear modulus of PIPD. Polymer, 2005, 46, 9144-9154.	1.8	18
70	Work function anisotropy and surface stability of half-metallicCrO2. Physical Review B, 2008, 77, .	1.1	18
71	Reversed spin polarization at the Co(001)-HfO2(001) interface. Physical Review B, 1998, 58, 15422-15425.	1.1	15
72	Lattice and local-mode vibrations in anhydrous and protonized LiMn2O4 spinels from first-principles theory. Journal of Materials Chemistry, 2007, 17, 4908.	6.7	15

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73	Theoretical Study of the Stable Radicals Galvinoxyl, Azagalvinoxyl and Wursterâ€™s Blue Perchlorate in the Solid State. Journal of Physical Chemistry A, 2008, 112, 7734-7738.	1.1	15
74	Intrinsic defects and dopants in LiNH2: a first-principles study. Physical Chemistry Chemical Physics, 2011, 13, 6043.	1.3	15
75	NMR shieldings from density functional perturbation theory: GIPAW versus all-electron calculations. Journal of Chemical Physics, 2017, 146, 064115.	1.2	15
76	Nanometre superstructure in liquid alkali-thallium alloys. Journal of Physics Condensed Matter, 1993, 5, 9253-9260.	0.7	14
77	Native Defects and the Dehydrogenation of NaBH4. Journal of Physical Chemistry C, 2011, 115, 24429-24434.	1.5	13
78	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
79	Clusters in liquid K-Tl and Cs-Tl alloys. Journal of Physics Condensed Matter, 1994, 6, A255-A260.	0.7	12
80	First-principles modelling of magnesium titanium hydrides. Journal of Physics Condensed Matter, 2010, 22, 074208.	0.7	12
81	Switchable Fermi surface sheets in greigite. Physical Review B, 2012, 86, .	1.1	12
82	Carbon Support Effects on the Hydrogen Storage Properties of LiBH‹sub›4‹/sub› Nanoparticles: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 5102-5109.	1.5	12
83	Structural Studies of Polyaramid Fibers: Solid-State NMR and First-Principles Modeling. Macromolecules, 2016, 49, 5548-5560.	2.2	12
84	Band Offsets at the Interface between Crystalline and Amorphous Silicon from First Principles. Physical Review Applied, 2017, 8, .	1.5	12
85	Transport coefficients of liquids from first principles. Journal of Non-Crystalline Solids, 1999, 250-252, 82-90.	1.5	11
86	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.	1.4	11
87	Preactive Site in Zieglerâ€“Natta Catalysts. Journal of Physical Chemistry C, 2019, 123, 14490-14500.	1.5	11
88	Theoretical models of Rashba spin splitting in asymmetric SrTiO3 -based heterostructures. Physical Review B, 2017, 95, .	1.1	10
89	Interrelation of Work Function and Surface Stability: The Case of BaAl4. Chemistry of Materials, 2005, 17, 3879-3882.	3.2	9
90	Model for the Formation Energies of Alanates and Boranates. Journal of Physical Chemistry C, 2007, 111, 9592-9594.	1.5	9

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91	Excess manganese as the origin of the low-temperature anomaly in NiMnSb. Physical Review B, 2013, 88, .	1.1	9
92	Impact of F and S doping on (Mn,Fe)2(P,Si) giant magnetocaloric materials. Acta Materialia, 2022, 234, 118057.	3.8	9
93	Structure of liquid caesium-lead alloys. Journal of Non-Crystalline Solids, 1993, 156-158, 34-37.	1.5	8
94	Publisher's Note: Modeling and analysis of the three-dimensional current density in sandwich-type single-carrier devices of disordered organic semiconductors [Phys. Rev. B79, 085203 (2009)]. Physical Review B, 2009, 79, .	1.1	8
95	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.	0.7	7
96	Generalised coexistence of a low work function and a stable surface: CaAl4 and BaAuIn3. Surface Science, 2006, 600, 2495-2500.	0.8	7
97	Lithium trapping by excess oxygen inWO3:A first-principles study. Physical Review B, 2000, 62, 1508-1511.	1.1	6
98	Quantum confinement and band offsets in amorphous silicon quantum wells. Physical Review B, 2014, 90, .	1.1	6
99	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.	1.4	6
100	Energy, metastability, and optical properties of anion-disordered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>R</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mo>â^'</mml:mo><mml:mn>2</mml:mn><mml:mi>x</mml:mi> <mml:math		

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109	Quantum mechanics calculations on the diastereomeric salts of cyclic phosphoric acids with ephedrine. Computational and Theoretical Chemistry, 2005, 717, 205-214.	1.5	0
110	q-GRID: a new method to calculate lattice and interaction energies for molecular crystals from electron densities. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s348-s348.	0.0	0
111	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