Heike C Herper

List of Publications by Year
in descending order

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80 papers	1,870 citations	394390 19 h-index	276858 41 g-index
85 all docs	85 docs citations	85 times ranked	1788 citing authors

#	Article	IF	Citations
1	Ab initiofull-potential study of the structural and magnetic phase stability of iron. Physical Review B, 1999, 60, 3839-3848.	3.2	337
2	Modelling the phase diagram of magnetic shape memory Heusler alloys. Journal Physics D: Applied Physics, 2006, 39, 865-889.	2.8	306
3	First-principles and Monte Carlo study of magnetostructural transition and magnetocaloric properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ni</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn> Physical Review B, 2010, 81, .	3.2	119
4	Designing shape-memory Heusler alloys from first-principles. Applied Physics Letters, 2011, 99, .	3.3	91
5	Complex magnetic ordering as a driving mechanism of multifunctional properties of Heusler alloys from first principles. European Physical Journal B, 2013, 86, 1.	1.5	88
6	Graphene as a Reversible Spin Manipulator of Molecular Magnets. Physical Review Letters, 2011, 107, 257202.	7.8	68
7	A Firstâ€Principles Investigation of the Compositional Dependent Properties of Magnetic Shape Memory Heusler Alloys. Advanced Engineering Materials, 2012, 14, 530-546.	3.5	54
8	Influence of Electron Correlation on the Electronic Structure and Magnetism of Transition-Metal Phthalocyanines. Journal of Chemical Theory and Computation, 2016, 12, 1772-1785.	5.3	54
9	Elucidating the 3d Electronic Configuration in Manganese Phthalocyanine. Journal of Physical Chemistry A, 2014, 118, 927-932.	2.5	43
10	Fundamental Aspects of Magnetic Shape Memory Alloys: Insights from <i>Ab Initio</i> and Monte Carlo Studies. Materials Science Forum, 0, 635, 3-12.	0.3	41
11	Oxygen-tuned magnetic coupling of Fe-phthalocyanine molecules to ferromagnetic Co films. Physical Review B, 2013, 88, .	3.2	41
12	Composition-Dependent Basics of Smart Heusler Materials from First- Principles Calculations. Materials Science Forum, 0, 684, 1-29.	0.3	39
13	Microscopic theory of the martensitic transition inFe1â^'xNix. Physical Review B, 1993, 47, 5589-5596.	3.2	37
14	Local atomic order and element-specific magnetic moments of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub> films on MgO(001) and GaAs(001) substrates. Physical Review B, 2009, 80, .	3.2	35
15	High-throughput and data-mining approach to predict new rare-earth free permanent magnets. Physical Review B, 2020, 101, .	3.2	34
16	Iron porphyrin molecules on Cu(001): Influence of adlayers and ligands on the magnetic properties. Physical Review B, 2013, 87, .	3.2	33
17	Basic Properties of Magnetic Shape-Memory Materials from First-Principles Calculations. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2012, 43, 2891-2900.	2.2	28
18	Electronic structure of the austenitic and martensitic state of magnetocaloric Ni-Mn-In Heusler alloy films. Physical Review B, 2013, 88, .	3.2	28

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19	Electric transport in Fe/ZnSe/Fe heterostructures. Physical Review B, 2001, 64, .	3.2	27
20	Fe phthalocyanine on Co(001): Influence of surface oxidation on structural and electronic properties. Physical Review B, 2014, 89, .	3.2	24
21	Interlayer exchange coupling and perpendicular electric transport in Fe/Si/Fe trilayers. Physical Review B, 2002, 66, .	3.2	21
22	Ni-based Heusler compounds: How to tune the magnetocrystalline anisotropy. Physical Review B, 2018, 98, .	3.2	21
23	Influence of the interlayer exchange coupling on the electric transport in Fe/Cr/Fe andFe/Cr/T/Fe(T=Mn,V): Anab initiostudy. Physical Review B, 2003, 68, .	3.2	18
24	Electron Correlation Effects in the Fe Dimer. Journal of Physical Chemistry A, 2006, 110, 10799-10804.	2.5	18
25	On the rich magnetic phase diagram of (Ni, Co)â€“Mnâ€“Sn Heusler alloys. Journal Physics D: Applied Physics, 2016, 49, 395001.	2.8	18
26	Understanding iron and its alloys from first principles. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 2000, 80, 141-153.	0.6	17
27	Induced magnetism on silicon in Fe<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>Si quasi-Heusler compound. Physical Review B, 2012, 85, .	3.2	17
28	Combining electronic structure and many-body theory with large databases: A method for predicting the nature of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi></mml:mrow></mml:m states in Ce compounds. Physical Review Materials, 2017, 1, .	2.4	16
29	The Invar Property of Elemental F.C.C. Co and Large Spontaneous Magnetostriction of B.C.C. Fe-Co. Physica Status Solidi (B): Basic Research, 1999, 214, 175-185.	1.5	13
30	Large-scale molecular-dynamics simulations of martensitic nucleation and shape-memory effects in transition metal alloys. Phase Transitions, 1998, 65, 79-108.	1.3	12
31	Computational screening of Fe-Ta hard magnetic phases. Physical Review B, 2020, 101, .	3.2	11
32	Induced magnetic Cu moments and magnetic ordering in Cu₂MnAl thin films on MgO(0â€‰0â€‰1) observed by XMCD. Journal Physics D: Applied Physics, 2011, 44, 415004.	2.8	9
33	Atomic contributions to the valence band photoelectron spectra of metal-free, iron and manganese phthalocyanines. Journal of Electron Spectroscopy and Related Phenomena, 2015, 205, 92-97.	1.7	9
34	Data-driven design of a new class of rare-earth free permanent magnets. Acta Materialia, 2021, 212, 116913.	7.9	9
35	Co2+xFe1â^'xSi/MgO(001) Heusler alloys: Influence of off-stoichiometry and lattice distortion on the magnetic properties in bulk and on MgO(001). Journal of Applied Physics, 2011, 109, .	2.5	8
36	Ab Initio Study of Iron and Cr/Fe(001). Phase Transitions, 2002, 75, 185-193.	1.3	7

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37	Ab initiostudy of the interface properties of Fe/GaAs(110). Physical Review B, 2009, 80, .	3.2	7
38	First-principles investigations of caloric effects in ferroic materials. , 2012, , .		6
39	Phase Diagrams of Conventional and Inverse Functional Magnetic Heusler Alloys: New Theoretical and Experimental Investigations. Springer Series in Materials Science, 2012, , 19-47.	0.6	6
40	A first-principles study aided with Monte Carlo simulations of carbon doped iron-manganese alloys. European Physical Journal B, 2012, 85, 1.	1.5	6
41	Element-specific electronic structure and magnetic properties of an epitaxialNi51.6Mn32.9Sn15.5thin film at the austenite-martensite transition. Physical Review B, 2015, 91, .	3.2	6
42	Ligand Effects on the Linear Response Hubbard U: The Case of Transition Metal Phthalocyanines. Journal of Physical Chemistry A, 2019, 123, 3214-3222.	2.5	6
43	The CeFe₁₁Ti permanent magnet: a closer look at the microstructure of the compound. Journal of Physics Condensed Matter, 2019, 31, 505505.	1.8	6
44	Ab-initio study of the electronic structure and magnetic properties of Ce2Fe17. Journal of Alloys and Compounds, 2021, 888, 161521.	5.5	6
45	Aspects of magnetotunnelling drawn fromab-initio-type calculations. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 2002, 82, 1027-1045.	0.6	5
46	Ab initiostudy of the electronic and magnetic structure of the TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>rutile (110)/Fe interface. Physical Review B, 2013, 88, .	3.2	5
47	Influence of ligands on the electronic and magnetic properties of Fe porphyrin in gas phase and on Cu(001). Journal of Applied Physics, 2015, 117, 17B318.	2.5	5
48	Localized versus itinerant character of 4f-states in cerium oxides. Journal of Physics Condensed Matter, 2020, 32, 215502.	1.8	5
49	Perpendicular electric transport in Fe/X/Fe model heterostructures. Journal of Applied Physics, 2002, 91, 8777.	2.5	4
50	Ab initio investigation of intermixing effects of Cr on BCC Fe(001). Journal of Magnetism and Magnetic Materials, 2002, 240, 401-403.	2.3	4
51	Theory of electric transport through Fe/V/Fe trilayers including the effect of impurities. Physica Status Solidi (B): Basic Research, 2005, 242, 271-277.	1.5	4
52	Suitability of Fe/GaAs and (Co,Ni)Mn(Ga,Ge) for Spintronics Applications: An Ab Initio Study. IEEE Transactions on Magnetics, 2009, 45, 3965-3968.	2.1	4
53	Realistic first-principles calculations of the magnetocaloric effect: applications to hcp Gd. Materials Research Letters, 2022, 10, 156-162.	8.7	4
54	Perpendicular transport in Fe/InP/Fe heterostructures. Journal of Magnetism and Magnetic Materials, 2002, 240, 180-182.	2.3	3

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55	Ab Initio Study of Electric Transport and Interlayer Exchange Coupling in Fe-Si-Fe Systems. Phase Transitions, 2003, 76, 523-532.	1.3	3
56	CPP transport in Fe/Cr/Fe trilayers with mn impurities: anab initiostudy. Phase Transitions, 2004, 77, 191-200.	1.3	2
57	Influence of domain wall scattering on the magnetoresistance of Co andCo80Pt20film systems. Physical Review B, 2008, 77, .	3.2	2
58	Magnetic properties of ultrathin Fe₃Si films on GaAs(001). Journal of Physics: Conference Series, 2010, 200, 072105.	0.4	2
59	Ferromagnetic Heusler Alloy Thin Films: Electronic Properties and Magnetic Moment Formation. Springer Tracts in Modern Physics, 2013, , 119-162.	0.1	2
60	Tuning the Magnetic Anisotropy of NiPtMnGa by Substitution and Epitaxial Strain. IEEE Transactions on Magnetics, 2019, 55, 1-4.	2.1	2
61	AB Initio Investigations of Phonon Anomalies and Martensitic Transformations. , 1997, , 213-218.		2
62	Chemical Switching of the Magnetic Coupling in a MnPc Dimer by Means of Chemisorption and Axial Ligands. Journal of Physical Chemistry C, 2020, 124, 27185-27193.	3.1	2
63	Electric transport perpendicular to the planes. Physica Status Solidi (B): Basic Research, 2006, 243, 2632-2642.	1.5	1
64	Domain walls in systems with large magneto-crystalline anisotropy. Phase Transitions, 2006, 79, 827-837.	1.3	1
65	A comparative study of (Fe, Fe₃Si)/GaAs and Heusler/MgO for spintronics applications. Journal of Physics: Conference Series, 2010, 200, 072038.	0.4	1
66	An ab initio perspective on scanning tunneling microscopy measurements of the tunable Kondo resonance of the TbPc2 molecule on a gold substrate. Physical Review B, 2020, 101, .	3.2	1
67	Tuning the magnetic phase diagram of Ni-Mn-Ga by Cr and Co substitution. Journal Physics D: Applied Physics, 0, , .	2.8	1
68	Electronic Structure of Isolated Molecules. SpringerBriefs in Applied Sciences and Technology, 2020, , 25-34.	0.4	1
69	Interaction with Substrates. SpringerBriefs in Applied Sciences and Technology, 2020, , 45-64.	0.4	1
70	Influence of antiphase boundary of the MnAl Ï„ -phase on the energy product. Physical Review Materials, 2019, 3, .	2.4	1
71	Structure and Magnetism of Iron in Fe/Pd Multilayers. Phase Transitions, 2002, 75, 125-132.	1.3	0
72	Ab initio study of CPP transport in Fe/Cr/Fe trilayers: influence of transition metal impurities. Materials Research Society Symposia Proceedings, 2002, 746, 1.	0.1	0

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73	Magnetism and magnetoresistance in Fe/Cr/V/Cr/Fe. Phase Transitions, 2005, 78, 169-177.	1.3	0
74	First-principles calculations of the magnetoresistance of Fe/V trilayers and multilayers. Phase Transitions, 2005, 78, 827-837.	1.3	0
75	Magnetic Phase Diagram of Transition Metal Doped ZnO from Density Functional Theory Calculations and Monte Carlo Simulations. Materials Research Society Symposia Proceedings, 2010, 1260, 1.	0.1	0
76	Ab-initio modeling of Fe-Mn based alloys and nanoclusters. Materials Research Society Symposia Proceedings, 2011, 1296, 1.	0.1	0
77	Deposited Transition Metalâ€Centered Porphyrin and Phthalocyanine Molecules: Influence of the Substrates on the Magnetic Properties. , 0, , .		0
78	Electron Correlation and Spin Transition. SpringerBriefs in Applied Sciences and Technology, 2020, , 35-43.	0.4	0
79	Theoretical Methods. SpringerBriefs in Applied Sciences and Technology, 2020, , 19-24.	0.4	0
80	Domain Wall Formation in Ferromagnetic Layers: An Ab Initio Study. , 2008, , 269-280.		0