

Markus E Gruner

List of Publications by Year in descending order

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131
papers

3,975
citations

126901

33
h-index

138468

58
g-index

139
all docs

139
docs citations

139
times ranked

2976
citing authors

#	ARTICLE	IF	CITATIONS
1	Modelling the phase diagram of magnetic shape memory Heusler alloys. Journal Physics D: Applied Physics, 2006, 39, 865-889.	2.8	306
2	Mastering hysteresis in magnetocaloric materials. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20150308.	3.4	210
3	Monte Carlo study of the influence of antiferromagnetic exchange interactions on the phase transitions of ferromagnetic Ni-Mn-X alloys		

#	ARTICLE	IF	CITATIONS
19	Shape Memory Alloys: A Summary of Recent Achievements. Materials Science Forum, 0, 583, 21-41.	0.3	64
20	Ab initio studies of effect of copper substitution on the electronic and magnetic properties of Ni ₂ MnGa and Mn ₂ NiGa. Physical Review B, 2013, 88, .	3.2	60
21	A First-Principles Investigation of the Compositional Dependent Properties of Magnetic Shape Memory Heusler Alloys. Advanced Engineering Materials, 2012, 14, 530-546.	3.5	54
22	Magnetocaloric materials for refrigeration near room temperature. MRS Bulletin, 2018, 43, 269-273.	3.5	50
23	Modulations in martensitic Heusler alloys originate from nanotwin ordering. Scientific Reports, 2018, 8, 8489.	3.3	47
24	Optimization of smart Heusler alloys from first principles. Journal of Alloys and Compounds, 2013, 577, S107-S112.	5.5	46
25	Lattice dynamics and structural stability of ordered Fe ₃ Co ₄₅ Heusler alloys. Physical Review B, 2010, 81, .	3.2	45
26	Impact of lattice dynamics on the phase stability of metamagnetic FeRh: Bulk and thin films. Physical Review B, 2016, 94, .	3.2	44
27	Modeling Structural and Magnetic Phase Transitions in Iron-Nickel Nanoparticles. Phase Transitions, 2003, 76, 355-365.	1.3	42
28	Ab initio investigation of twin boundary motion in the magnetic shape memory Heusler alloy Ni ₂ MnGa. Journal of Materials Science, 2008, 43, 3825-3831.	3.7	41
29	Fundamental Aspects of Magnetic Shape Memory Alloys: Insights from Ab Initio and Monte Carlo Studies. Materials Science Forum, 0, 635, 3-12.	0.3	41
30	The ferromagnetic shape memory system Fe _{1-x} Pd _x Cu. Acta Materialia, 2010, 58, 5949-5961.	7.9	39
31	Composition-Dependent Basics of Smart Heusler Materials from First-Principles Calculations. Materials Science Forum, 0, 684, 1-29.	0.3	39
32	First-principles studies on graphene-supported transition metal clusters. Journal of Chemical Physics, 2014, 141, 074707.	3.0	38
33	Effect of substitution on elastic stability, electronic structure and magnetic property of Ni _{1-x} Mn _x based Heusler alloys: An ab initio comparison. Journal of Alloys and Compounds, 2015, 632, 822-829.	5.5	38
34	Interacting magnetic clusters, spin glasses and strain glasses in Ni _{1-x} Mn _x based Heusler structured intermetallics. Physica Status Solidi (B): Basic Research, 2014, 251, 2135-2148.	1.5	37
35	Electronic structure and lattice dynamics of the magnetic shape-memory alloy Co ₂ Cr ₃ Heusler alloy. Physical Review B, 2010, 82, .	3.2	36
36	Achieving large magnetocaloric effects in Co- and Cr-substituted Heusler alloys: Predictions from first-principles and Monte Carlo studies. Physical Review B, 2015, 91, .	3.2	36

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37	Scaling study and thermodynamic properties of the cubic helimagnet FeGe. Physical Review B, 2016, 94, .	3.2	34
38	Simulating functional magnetic materials on supercomputers. Journal of Physics Condensed Matter, 2009, 21, 293201.	1.8	33
39	Anisotropic ferromagnetism in carbon-doped zinc oxide from first-principles studies. Physical Review B, 2012, 86, .	3.2	31
40	Large thermopower anisotropy in PdCoO_2 thin films. Physical Review Materials, 2019, 3, .	2.4	31
41	Impact of local lattice distortions on the structural stability of Fe-Pd magnetic shape-memory alloys. Physical Review B, 2011, 83, .	3.2	30
42	Ordering tendencies and electronic properties in quaternary Heusler derivatives. Physical Review B, 2017, 96, .	3.2	29
43	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
44	First-principles investigations of multimetallic transition metal clusters. Philosophical Magazine, 2008, 88, 2725-2738.	1.6	27
45	Competing structural ordering tendencies in Heusler-type alloys with high Curie temperatures: $\text{Fe}_2\text{Mn}_2\text{Ti}$. Physical Review B, 2010, 82, .	3.2	27
46	Magnetic Nanostructures by Adaptive Twinning in Strained Epitaxial Films. Physical Review Letters, 2011, 107, 206105.	7.8	27
47	Large-scale ab initio simulations of binary transition metal clusters for storage media materials. Journal of Physics Condensed Matter, 2009, 21, 064228.	1.8	26
48	Magnetoelastic coupling and the formation of adaptive martensite in magnetic shape memory alloys. Physica Status Solidi (B): Basic Research, 2014, 251, 2067-2079.	1.5	26
49	High Thermopower with Metallic Conductivity in <i>p</i> -Type Li-Substituted PbPdO_2 . Chemistry of Materials, 2016, 28, 3367-3373.	6.7	25
50	Properties and Decomposition of Heusler Alloys. Energy Technology, 2018, 6, 1478-1490.	3.8	24
51	The metamagnetic behavior and giant inverse magnetocaloric effect in $\text{NiCoMn}(\text{Ga, In, Sn})$ Heusler alloys. Journal of Magnetism and Magnetic Materials, 2015, 385, 193-197.	2.3	22
52	Tailoring magnetic frustration in strained epitaxial FeRh films. Physical Review B, 2016, 93, .	3.2	22
53	Preparation and properties of nanostructured magnetic hollow microspheres: experiment and simulation. Phase Transitions, 2005, 78, 741-750.	1.3	21
54	Effect of temperature and compositional changes on the phonon properties of Ni-Mn-Ga shape memory alloys. Physical Review B, 2012, 86, .	3.2	21

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55	Interaction of Phase Transformation and Magnetic Properties of Heusler Alloys: A Density Functional Theory Study. <i>Jom</i> , 2013, 65, 1540-1549.	1.9	21
56	Impact of strain-induced electronic topological transition on the thermoelectric properties of PtCoO_2 . <i>Physical Review B</i> , 2015, 92, .	3.2	20
57	Chemically ordered decahedral FePt nanocrystals observed by electron microscopy. <i>Physical Review B</i> , 2014, 89, .	2.8	19
58	Antiferromagnetism and segregation in cuboctahedral FePt nanoparticles. <i>Journal Physics D: Applied Physics</i> , 2008, 41, 134015.	2.8	19
59	Interplay of phase sequence and electronic structure in the modulated martensites of Mn_2Pt from first-principles calculations. <i>Physical Review B</i> , 2017, 96, .	2.0	18
60	Competition between ordering, twinning, and segregation in binary magnetic $3d-5d$ nanoparticles: A supercomputing perspective. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 277-288.	3.2	18
61	Microscopic nonequilibrium energy transfer dynamics in a photoexcited metal/insulator heterostructure. <i>Physical Review B</i> , 2019, 100, .	2.8	17
62	Chemical trends in structure and magnetism of bimetallic nanoparticles from atomistic calculations. <i>Journal Physics D: Applied Physics</i> , 2010, 43, 474008.	1.5	16
63	Monte Carlo simulations of high-moment - low-moment transitions in Invar alloys. <i>European Physical Journal B</i> , 1998, 2, 107-119.	2.6	16
64	Influence of magnetism on the structural stability of cubic $\text{L21Ni}_2\text{MnGa}$. <i>European Physical Journal: Special Topics</i> , 2008, 158, 193-198.	3.5	16
65	Understanding the Magnetic Shape Memory System FePd_x by Thin Film Experiments and First Principle Calculations. <i>Advanced Engineering Materials</i> , 2012, 14, 724-749.	3.2	15
66	Influence of hydrogenation on the vibrational density of states of magnetocaloric LaFeSi_2 . <i>Physical Review B</i> , 2020, .	5.6	14
67	Magnetic-field-induced changes in magnetic shape memory alloys. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2008, 481-482, 258-261.	0.4	14
68	Core-shell morphologies of FePt and CoPt nanoparticles: An <i>ab initio</i> comparison. <i>Journal of Physics: Conference Series</i> , 2010, 200, 072039.	0.6	14
69	Domain Structure in the Tetragonal Phase of BaTiO_3 from Bulk to Nanoparticles. <i>Ferroelectrics</i> , 2012, 426, 21-30.	1.5	14
70	Moment-Volume Coupling in $\text{La}(\text{Fe}_{1-x}\text{Si}_x)_{13}$. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1700465.	1.5	14
71	Determining the vibrational entropy change in the giant magnetocaloric material LaFeSi_2 by nuclear resonant inelastic x-ray scattering. <i>Physical Review B</i> , 2018, 98, .	2.3	13
72	Structure and magnetism of near-stoichiometric FePd nanoparticles. <i>Journal of Magnetism and Magnetic Materials</i> , 2009, 321, 861-864.		

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73	Enhancing magnetocrystalline anisotropy of the Fe ₇₀ Pd ₃₀ magnetic shape memory alloy by adding Cu. Acta Materialia, 2012, 60, 6920-6930.	7.9	13
74	Role of the exchange-correlation functional on the structural, electronic, and optical properties of cubic and tetragonal SrTiO_3 including many-body effects. Physical Review Materials, 2019, 3, .	2.4	13
75	Structural and magnetic properties of ternary Fe _{1-x} Mn _x Pt nanoalloys from first principles. Beilstein Journal of Nanotechnology, 2011, 2, 162-172.	2.8	12
76	Segregation tendency of Heusler alloys. Physical Review Materials, 2019, 3, .	2.4	12
77	Probing Structural and Magnetic Instabilities and Hysteresis in Heuslers by Density Functional Theory Calculations. Physica Status Solidi (B): Basic Research, 2018, 255, 1700296.	1.5	11
78	Compositional trends and magnetic excitations in binary and ternary Fe _{1-x} Pd _x magnetic shape memory alloys. Journal of Alloys and Compounds, 2013, 577, S333-S337.	5.5	10
79	Electronic structure and magnetism of epitaxial Ni _{1-x} Mn _x Ga(-Co) thin films with partial disorder: a view across the phase transition. Journal Physics D: Applied Physics, 2017, 50, 465005.	2.8	10
80	Ab initio modeling of martensitic transformations (MT) in magnetic shape memory alloys. Journal of Magnetism and Magnetic Materials, 2007, 310, 2761-2763.	2.3	9
81	First-principles study of the structural stability of L1 ₂ order in Pt-based alloys. Journal of Physics: Conference Series, 2010, 200, 072021.	0.4	9
82	Optimizing the Magnetocaloric Effect in Ni _{1-x} Mn _x Sn by Substitution: A First-Principles Study. IEEE Transactions on Magnetics, 2014, 50, 1-4.	2.1	9
83	Effective decoupling of ferromagnetic sublattices by frustration in Heusler alloys. Physical Review B, 2022, 105, .	3.2	9
84	Theoretical description of optical and x-ray absorption spectra of MgO including many-body effects. Physical Review B, 2021, 103, .	3.2	8
85	Structural and Magnetic Properties of Transition Metal Nanoparticles from First Principles. , 2008, , 117-128.		8
86	Simulation of the (p, T) phase diagram of the temperature-driven metamagnet $\text{Fe}_{1-x}\text{Rh}_x$. Phase Transitions, 2005, 78, 209-217.	1.3	7
87	Dynamics of optical excitations in a Fe/MgO(001) heterostructure from time-dependent density functional theory. Physical Review B, 2019, 99, .	3.2	7
88	Magnetic properties of nanostructured hollow microspheres. Journal of Magnetism and Magnetic Materials, 2007, 310, 2453-2455.	2.3	6
89	First-principles investigations of caloric effects in ferroic materials. , 2012, , .		6
90	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

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91	Trends in spin and orbital magnetism of free and encapsulated FePt nanoparticles. Physica Status Solidi (A) Applications and Materials Science, 2013, 210, 1282-1297.	1.8	6
92	Tuning the Thermoelectric Properties of Transition Metal Oxide Thin Films and Superlattices on the Quantum Scale. Physica Status Solidi (B): Basic Research, 2022, 259, 2100270.	1.5	6
93	Impact of local arrangement of Fe and Ni on the phase stability and magnetocrystalline anisotropy in Fe-Ni-Al Heusler alloys. Physical Review Materials, 2022, 6, .	2.4	6
94	HR-TEM Studies of FePt Nanoparticles by Exit Wave Reconstruction. Materials Research Society Symposia Proceedings, 2007, 998, 1.	0.1	5
95	First-Principles Calculations of Magnetic Properties of Cr-Doped Ni ₄₅ Co ₅ Mn ₃₇ In ₁₃ Heusler Alloys. IEEE Transactions on Magnetics, 2015, 51, 1-4.	2.1	5
96	Epitaxial strain adaptation in chemically disordered FeRh thin films. Physical Review B, 2019, 99, .	3.2	5
97	Magnetism of close packed Fe ₁₄₇ clusters. Phase Transitions, 2006, 79, 701-707.	1.3	4
98	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
99	Absence of ferromagnetic interaction in Co-Co nearest neighbor impurity pairs in ZnO: An analysis from GGA+U studies. , 2012, , .		4
100	Electronic and magnetic trends in martensitically transforming Fe-Pd alloys. Journal of Magnetism and Magnetic Materials, 2012, 324, 3524-3529.	2.3	4
101	First-Principles and Monte Carlo Studies of Magnetocaloric Effects. Advances in Science and Technology, 2016, 97, 124-133.	0.2	4
102	Interface-related magnetic and vibrational properties in Fe/MgO heterostructures from nuclear resonant spectroscopy and first-principles calculations. Physical Review Materials, 2020, 4, .	2.4	4
103	Effect of lattice excitations on transient near-edge x-ray absorption spectroscopy. Physical Review B, 2021, 104, .	3.2	4
104	Possible one-dimensional structures obtained from transition metal atom doped silicon nanoclusters. Phase Transitions, 2006, 79, 709-716.	1.3	3
105	Simulating Structure, Magnetism and Electronic Properties of Monoatomic, Binary and Ternary Transition Metal Nanoclusters. , 2008, , .		3
106	First-principles study of ferromagnetic Ni ₂ CoGa(Zn) alloys in the Heusler and the inverse Heusler structure. Materials Research Society Symposia Proceedings, 2009, 1200, 50.	0.1	3
107	New Functional Magnetic Shape Memory Alloys from First-Principles Calculations. Materials Research Society Symposia Proceedings, 2009, 1200, 38.	0.1	3
108	Magnetic States of the Ni _{1.75} Co _{0.25} Mn _{1.25} Cr _{0.25} In _{1.25} Heusler Alloy. IEEE Transactions on Magnetics, 2015, 51, 1-4.		

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109	Characterization of new ferromagnetic Fe-Co-Zn-Ga alloys by ab initio investigations. , 2009, , .		3
110	Chemical long range ordering in all-d-metal Heusler alloys. Journal of Applied Physics, 2022, 131, .	2.5	3
111	Monte Carlo simulations of magnetovolume instabilities in anti-Invar systems. Computational Materials Science, 1998, 10, 230-234.	3.0	2
112	High-Moment-Low-Moment Description of Magnetovolume Effects in $Y(\text{Mn}_x\text{Al}_{1-x})_2$ and $Y_x\text{Sc}_{1-x}\text{Mn}_2$. Phase Transitions, 2002, 75, 221-230.	1.3	2
113	First-principles study of static displacements in Fe-Pd magnetic shape-memory alloys. Materials Research Society Symposia Proceedings, 2009, 1200, 57.	0.1	2
114	Structural ordering tendencies in the new ferromagnetic NiCoFeGaZn Heusler alloys. Physics Procedia, 2010, 10, 144-148.	1.2	2
115	Large magnetocaloric effects in magnetic intermetallics: First-principles and Monte Carlo studies. MATEC Web of Conferences, 2015, 33, 02001.	0.2	2
116	Probing Structural and Magnetic Instabilities and Hysteresis in Heuslers by Density Functional Theory Calculations (Phys. Status Solidi B 2/2018). Physica Status Solidi (B): Basic Research, 2018, 255, 1870108.	1.5	2
117	$Z \hat{A} T_j \text{ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 427 Td}$	2.3	2
118	Anisotropic carrier dynamics in a laser-excited $\text{Fe}_{1-x}\text{Mn}_x$ heterostructure from real-time time-dependent density functional theory. Physical Review B, 2022, 105, .	3.2	2
119	Simulation of Magnetovolume Effects in $\text{Fe}_{65}\text{Ni}_{35}$ Nanoparticles. Progress of Theoretical Physics Supplement, 2000, 138, 154-155.	0.1	1
120	A first-principles study of the martensitic instabilities in magnetic shape memory alloys. Materials Research Society Symposia Proceedings, 2007, 1050, 1.	0.1	1
121	A comparative study of $(\text{Fe}, \text{Fe}_3\text{Si})/\text{GaAs}$ and Heusler/MgO for spintronics applications. Journal of Physics: Conference Series, 2010, 200, 072038.	0.4	1
122	Magnetic Interactions Governing the Inverse Magnetocaloric Effect in Martensitic NiMn -Based Shape-memory Alloys. Springer Series in Materials Science, 2012, , 67-77.	0.6	1
123	Probing Glassiness in Heuslers via Density Functional Theory Calculations. Springer Series in Materials Science, 2018, , 153-182.	0.6	1
124	MONTE CARLO STUDY OF THE MAGNETOELASTIC PROPERTIES OF FE-NI CLUSTERS. , 2000, , .		1
125	Domain formation in hollow spherical Invar nano-particles. Phase Transitions, 2005, 78, 711-721.	1.3	0
126	Structure, lattice dynamics and Fermi surface of the magnetic shape memory system CoNiGa from first principles calculations. Physics Procedia, 2010, 10, 138-143.	1.2	0

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127	From Tiny Magnetic Clusters to Functional Magnetic Materials. , 2011, , .		0
128	Ab-initio modeling of Fe-Mn based alloys and nanoclusters. Materials Research Society Symposia Proceedings, 2011, 1296, 1.	0.1	0
129	Martensitic Transformations of Ni ^x Mn ^{1-x} Heusler Alloys with X=Ga, In and Sn. Minerals, Metals and Materials Series, 2018, , 185-188.	0.4	0
130	Nucleation, Structure and Magnetism of Transition Metal Clusters from First Principles. Nanoscience and Technology, 2012, , 77-98.	1.5	0
131	Electronic and Vibrational Properties of Fe ₂ NiAl and Co ₂ NiAl Full Heusler Alloys: A First-Principles Comparison. IEEE Transactions on Magnetism, 2022, 58, 1-5.	2.1	0