

Markus E Gruner

List of Publications by Year in descending order

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131
papers

3,975
citations

145106

33
h-index

156644

58
g-index

139
all docs

139
docs citations

139
times ranked

3279
citing authors

#	ARTICLE	IF	CITATIONS
1	Tuning the Thermoelectric Properties of Transition Metal Oxide Thin Films and Superlattices on the Quantum Scale. <i>Physica Status Solidi (B): Basic Research</i> , 2022, 259, 2100270.	0.7	6
2	Magnetic and structural properties of Co-NiZr alloys. <i>Physical Review B</i> , 2022, 105, .	1.0	2
3	Electronic and Vibrational Properties of FeNi and CoNi Full Heusler Alloys: A First-Principles Comparison. <i>IEEE Transactions on Magnetics</i> , 2022, 58, 1-5.	1.2	0
4	Impact of local arrangement of Fe and Ni on the phase stability and magnetocrystalline anisotropy in Fe-Ni-Al Heusler alloys. <i>Physical Review Materials</i> , 2022, 6, .	0.9	6
5	Chemical long range ordering in all-d-metal Heusler alloys. <i>Journal of Applied Physics</i> , 2022, 131, .	1.1	3
6	Effective decoupling of ferromagnetic sublattices by frustration in Heusler alloys. <i>Physical Review B</i> , 2022, 105, .	1.1	9
7	Anisotropic carrier dynamics in a laser-excited Fe heterostructure from real-time time-dependent density functional theory. <i>Physical Review B</i> , 2022, 105, .	1.1	2
8	Theoretical description of optical and x-ray absorption spectra of MgO including many-body effects. <i>Physical Review B</i> , 2021, 103, .	1.1	8
9	Effect of lattice excitations on transient near-edge x-ray absorption spectroscopy. <i>Physical Review B</i> , 2021, 104, .	1.1	4
10	Influence of hydrogenation on the vibrational density of states of magnetocaloric LaFeSi thin films. <i>Physical Review B</i> , 2020, 102, .	1.1	15
11	Interface-related magnetic and vibrational properties in Fe/MgO heterostructures from nuclear resonant spectroscopy and first-principles calculations. <i>Physical Review Materials</i> , 2020, 4, .	0.9	4
12	Microscopic nonequilibrium energy transfer dynamics in a photoexcited metal/insulator heterostructure. <i>Physical Review B</i> , 2019, 100, .	1.1	18
13	Dynamics of optical excitations in a Fe/MgO(001) heterostructure from time-dependent density functional theory. <i>Physical Review B</i> , 2019, 99, .	1.1	7
14	Epitaxial strain adaptation in chemically disordered FeRh thin films. <i>Physical Review B</i> , 2019, 99, .	1.1	5
15	Role of the exchange-correlation functional on the structural, electronic, and optical properties of cubic and tetragonal SrTiO_3 including many-body effects. <i>Physical Review Materials</i> , 2019, 3, .	0.9	13
16	Segregation tendency of Heusler alloys. <i>Physical Review Materials</i> , 2019, 3, .	0.9	12
17	Large thermopower anisotropy in PdCoO_2 thin films. <i>Physical Review Materials</i> , 2019, 3, .	0.9	31
18	Martensitic Transformations of NiMnX Heusler Alloys with X=Ga, In and Sn. <i>Minerals, Metals and Materials Series</i> , 2018, , 185-188.	0.3	0

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19	Magnetocaloric materials for refrigeration near room temperature. MRS Bulletin, 2018, 43, 269-273.	1.7	50
20	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.	0.7	2
21	Moment-Volume Coupling in $\text{LaFe}_{1-x}\text{Si}_x$. Physica Status Solidi (B): Basic Research, 2018, 255, 1700465.	0.7	14
22	Probing Structural and Magnetic Instabilities and Hysteresis in Heuslers by Density Functional Theory Calculations. Physica Status Solidi (B): Basic Research, 2018, 255, 1700296.	0.7	11
23	Probing Glassiness in Heuslers via Density Functional Theory Calculations. Springer Series in Materials Science, 2018, , 153-182.	0.4	1
24	Modulations in martensitic Heusler alloys originate from nanotwin ordering. Scientific Reports, 2018, 8, 8489.	1.6	47
25	Determining the vibrational entropy change in the giant magnetocaloric material $\text{LaFe}_{11.6}\text{Si}_{1.4}$ by nuclear resonant inelastic x-ray scattering. Physical Review B, 2018, 98, .	1.4	14
26	Properties and Decomposition of Heusler Alloys. Energy Technology, 2018, 6, 1478-1490.	1.8	24
27	Hysteresis Design of Magnetocaloric Materials—From Basic Mechanisms to Applications. Energy Technology, 2018, 6, 1397-1428.	1.8	79
28	Electronic structure and magnetism of epitaxial $\text{NiMnGa}(-\text{Co})$ thin films with partial disorder: a view across the phase transition. Journal Physics D: Applied Physics, 2017, 50, 465005.	1.3	10
29	Ordering tendencies and electronic properties in quaternary Heusler derivatives. Physical Review B, 2017, 96, .	1.1	29
30	Interplay of phase sequence and electronic structure in the modulated martensites of Mn_2Pn from first-principles calculations. Physical Review B, 2017, 96, .	1.1	19
31	High Thermopower with Metallic Conductivity in p -Type Li-Substituted PbPdO_2 . Chemistry of Materials, 2016, 28, 3367-3373.	3.2	25
32	Scaling study and thermodynamic properties of the cubic helimagnet FeGe. Physical Review B, 2016, 94, .	1.1	34
33	Impact of lattice dynamics on the phase stability of metamagnetic FeRh: Bulk and thin films. Physical Review B, 2016, 94, .	1.1	44
34	Tailoring magnetic frustration in strained epitaxial FeRh films. Physical Review B, 2016, 93, .	1.1	22
35	Mastering hysteresis in magnetocaloric materials. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20150308.	1.6	210
36	Contradictory role of the magnetic contribution in inverse magnetocaloric Heusler materials. Physical Review B, 2016, 93, .	1.1	112

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37	First-Principles and Monte Carlo Studies of Magnetocaloric Effects. Advances in Science and Technology, 2016, 97, 124-133.	0.2	4
38	Achieving large magnetocaloric effects in Co- and Cr-substituted Heusler alloys: Predictions from first-principles and Monte Carlo studies. Physical Review B, 2015, 91, .	1.1	36
39	Impact of strain-induced electronic topological transition on the thermoelectric properties of PtCoO_2 . Physical Review B, 2015, 92, .	1.1	1
40	Large magnetocaloric effects in magnetic intermetallics: First-principles and Monte Carlo studies. MATEC Web of Conferences, 2015, 33, 02001.	0.1	2
41	Magnetic States of the $\text{Ni}_{1.75}\text{Co}_{0.25}\text{Mn}_{1.25}\text{Cr}_{0.25}\text{In}_{1.75}$ Heusler Alloy. IEEE Transactions on Magnetics, 2015, 51, 1-4.		
42	First-Principles Calculations of Magnetic Properties of Cr-Doped $\text{Ni}_{45}\text{Co}_5\text{Mn}_{37}\text{In}_{13}$ Heusler Alloys. IEEE Transactions on Magnetics, 2015, 51, 1-4.	1.2	5
43	The metamagnetic behavior and giant inverse magnetocaloric effect in Ni-Co-Mn (Ga, In, Sn) Heusler alloys. Journal of Magnetism and Magnetic Materials, 2015, 385, 193-197.	1.0	22
44	Effect of substitution on elastic stability, electronic structure and magnetic property of Ni-Mn based Heusler alloys: An ab initio comparison. Journal of Alloys and Compounds, 2015, 632, 822-829.	2.8	38
45	Element-Resolved Thermodynamics of Magnetocaloric $\text{LaFe}_{13}\text{MO}_7$. Physical Review Letters, 2015, 114, 057202.	2.9	78
46	First-principles studies on graphene-supported transition metal clusters. Journal of Chemical Physics, 2014, 141, 074707.	1.2	38
47	Optimizing the Magnetocaloric Effect in Ni-Mn-Sn by Substitution: A First-Principles Study. IEEE Transactions on Magnetics, 2014, 50, 1-4.	1.2	9
48	Chemically ordered decahedral FePt nanocrystals observed by electron microscopy. Physical Review B, 2014, 89, .	1.1	20
49	First-principles calculation of the instability leading to giant inverse magnetocaloric effects. Physical Review B, 2014, 89, .	1.1	73
50	Magnetoelastic coupling and the formation of adaptive martensite in magnetic shape memory alloys. Physica Status Solidi (B): Basic Research, 2014, 251, 2067-2079.	0.7	26
51	Interacting magnetic cluster spin glasses and strain glasses in Ni-Mn based Heusler structured intermetallics. Physica Status Solidi (B): Basic Research, 2014, 251, 2135-2148.	0.7	37
52	Trends in spin and orbital magnetism of free and encapsulated FePt nanoparticles. Physica Status Solidi (A) Applications and Materials Science, 2013, 210, 1282-1297.	0.8	6
53	Interaction of Phase Transformation and Magnetic Properties of Heusler Alloys: A Density Functional Theory Study. Jom, 2013, 65, 1540-1549.	0.9	21
54	Complex magnetic ordering as a driving mechanism of multifunctional properties of Heusler alloys from first principles. European Physical Journal B, 2013, 86, 1.	0.6	88

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55	Optimization of smart Heusler alloys from first principles. Journal of Alloys and Compounds, 2013, 577, S107-S112.	2.8	46
56	Compositional trends and magnetic excitations in binary and ternary FePdX magnetic shape memory alloys. Journal of Alloys and Compounds, 2013, 577, S333-S337.	2.8	10
57	Ab initio studies of effect of copper substitution on the electronic and magnetic properties of Ni ₂ MnGa and MnNiGa. Physical Review B, 2013, 88, .	1.1	60
58	First-principles investigations of caloric effects in ferroic materials. , 2012, , .		6
59	Absence of ferromagnetic interaction in Co-Co nearest neighbor impurity pairs in ZnO: An analysis from GGA+U studies. , 2012, , .		4
60	Phase Diagrams of Conventional and Inverse Functional Magnetic Heusler Alloys: New Theoretical and Experimental Investigations. Springer Series in Materials Science, 2012, , 19-47.	0.4	6
61	Anisotropic ferromagnetism in carbon-doped zinc oxide from first-principles studies. Physical Review B, 2012, 86, .	1.1	31
62	Effect of temperature and compositional changes on the phonon properties of Ni-Mn-Ga shape memory alloys. Physical Review B, 2012, 86, .	1.1	21
63	Electronic and magnetic trends in martensitically transforming FePd alloys. Journal of Magnetism and Magnetic Materials, 2012, 324, 3524-3529.	1.0	4
64	Enhancing magnetocrystalline anisotropy of the Fe ₇₀ Pd ₃₀ magnetic shape memory alloy by adding Cu. Acta Materialia, 2012, 60, 6920-6930.	3.8	13
65	Magnetic Interactions Governing the Inverse Magnetocaloric Effect in Martensitic NiMn-Based Shape-memory Alloys. Springer Series in Materials Science, 2012, , 67-77.	0.4	1
66	Competition between ordering, twinning, and segregation in binary magnetic 3d ⁵ d nanoparticles: A supercomputing perspective. International Journal of Quantum Chemistry, 2012, 112, 277-288.	1.0	18
67	Domain Structure in the Tetragonal Phase of BaTiO ₃ from Bulk to Nanoparticles. Ferroelectrics, 2012, 426, 21-30.	0.3	14
68	Understanding the Magnetic Shape Memory System FePdX by Thin Film Experiments and First Principle Calculations. Advanced Engineering Materials, 2012, 14, 724-749.	1.6	16
69	The Role of Adaptive Martensite in Magnetic Shape Memory Alloys. Advanced Engineering Materials, 2012, 14, 562-581.	1.6	99
70	A First-Principles Investigation of the Compositional Dependent Properties of Magnetic Shape Memory Heusler Alloys. Advanced Engineering Materials, 2012, 14, 530-546.	1.6	54
71	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.	1.1	28
72	Nucleation, Structure and Magnetism of Transition Metal Clusters from First Principles. Nanoscience and Technology, 2012, , 77-98.	1.5	0

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73	Structural and magnetic properties of ternary Fe _x Mn _x Pt nanoalloys from first principles. Beilstein Journal of Nanotechnology, 2011, 2, 162-172.	1.5	12
74	A guideline for atomistic design and understanding of ultrahard nanomagnets. Nature Communications, 2011, 2, 528.	5.8	67
75	Designing shape-memory Heusler alloys from first-principles. Applied Physics Letters, 2011, 99, .	1.5	91
76	From Tiny Magnetic Clusters to Functional Magnetic Materials. , 2011, , .		0
77	Impact of local lattice distortions on the structural stability of Fe-Pd magnetic shape-memory alloys. Physical Review B, 2011, 83, .	1.1	30
78	Magnetic Nanostructures by Adaptive Twinning in Strained Epitaxial Films. Physical Review Letters, 2011, 107, 206105.	2.9	27
79	Ab-initio modeling of Fe-Mn based alloys and nanoclusters. Materials Research Society Symposia Proceedings, 2011, 1296, 1.	0.1	0
80	First-principles study of the structural stability of L1 ₁ order in Pt-based alloys. Journal of Physics: Conference Series, 2010, 200, 072021.	0.3	9
81	A comparative study of (Fe, Fe ₃ Si)/GaAs and Heusler/MgO for spintronics applications. Journal of Physics: Conference Series, 2010, 200, 072038.	0.3	1
82	Chemical trends in structure and magnetism of bimetallic nanoparticles from atomistic calculations. Journal Physics D: Applied Physics, 2010, 43, 474008.	1.3	17
83	Competing structural ordering tendencies in Heusler-type alloys with high Curie temperatures: $\langle \text{Fe} \rangle \langle \text{Mn} \rangle^2 \langle \text{Mn} \rangle^2$ Physical Review B, 2010, 82, .	1.1	27
84	Structural ordering tendencies in the new ferromagnetic NiCoFeGaZn Heusler alloys. Physics Procedia, 2010, 10, 144-148.	1.2	2
85	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
86	The ferromagnetic shape memory system FePdCu. Acta Materialia, 2010, 58, 5949-5961.	3.8	39
87	Core-shell morphologies of FePt and CoPt nanoparticles: An ab initio comparison. Journal of Physics: Conference Series, 2010, 200, 072039.	0.3	14
88	Lattice dynamics and structural stability of ordered $\langle \text{Fe} \rangle \langle \text{Mn} \rangle^3 \langle \text{Mn} \rangle^2$ Physical Review B, 2010, 82, .	1.1	45
89	Electronic structure and lattice dynamics of the magnetic shape-memory alloy $\langle \text{Co} \rangle \langle \text{Mn} \rangle^2 \langle \text{Mn} \rangle^2$ Physical Review B, 2010, 82, .	1.1	36
90	Magnetic properties of small Pt-capped Fe, Co, and Ni clusters: A density functional theory study. Physical Review B, 2010, 82, .	1.1	68

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91	First-principles and Monte Carlo study of magnetostructural transition and magnetocaloric properties of Ni_2MnGa . Physical Review B, 2010, 81, .	1.1	119
92	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
93	First-principles study of static displacements in Fe-Pd magnetic shape-memory alloys. Materials Research Society Symposia Proceedings, 2009, 1200, 57.	0.1	2
94	New Functional Magnetic Shape Memory Alloys from First-Principles Calculations. Materials Research Society Symposia Proceedings, 2009, 1200, 38.	0.1	3
95	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.	1.2	4
96	Structure and magnetism of near-stoichiometric FePd nanoparticles. Journal of Magnetism and Magnetic Materials, 2009, 321, 861-864.	1.0	13
97	Surface energies of stoichiometric FePt and CoPt alloys and their implications for nanoparticle morphologies. Physical Review B, 2009, 80, .	1.1	121
98	Understanding the Phase Transitions of the Ni_2MnGa Shape Memory System from First Principles. Physical Review Letters, 2009, 102, 035702.	2.9	138
99	Simulating functional magnetic materials on supercomputers. Journal of Physics Condensed Matter, 2009, 21, 293201.	0.7	33
100	Large-scale ab initio simulations of binary transition metal clusters for storage media materials. Journal of Physics Condensed Matter, 2009, 21, 064228.	0.7	26
101	Characterization of new ferromagnetic Fe-Co-Zn-Ga alloys by ab initio investigations. , 2009, , .		3
102	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.	1.7	41
103	Magnetic-field-induced changes in magnetic shape memory alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2008, 481-482, 258-261.	2.6	14
104	Influence of magnetism on the structural stability of cubic L ₂ 1Ni ₂ MnGa. European Physical Journal: Special Topics, 2008, 158, 193-198.	1.2	16
105	Monte Carlo study of the influence of antiferromagnetic exchange interactions on the phase transitions of ferromagnetic Ni-Mn-X alloys.		

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109	Antiferromagnetism and segregation in cuboctahedral FePt nanoparticles. Journal Physics D: Applied Physics, 2008, 41, 134015.	1.3	19
110	Structural and Magnetic Properties of Transition Metal Nanoparticles from First Principles. , 2008, , 117-128.		8
111	A first-principles study of the martensitic instabilities in magnetic shape memory alloys. Materials Research Society Symposia Proceedings, 2007, 1050, 1.	0.1	1
112	HR-TEM Studies of FePt Nanoparticles by Exit Wave Reconstruction. Materials Research Society Symposia Proceedings, 2007, 998, 1.	0.1	5
113	Shellwise Mackay Transformation in Iron Nanoclusters. Physical Review Letters, 2007, 99, 083402.	2.9	80
114	Ab initio modeling of martensitic transformations (MT) in magnetic shape memory alloys. Journal of Magnetism and Magnetic Materials, 2007, 310, 2761-2763.	1.0	9
115	Magnetic properties of nanostructured hollow microspheres. Journal of Magnetism and Magnetic Materials, 2007, 310, 2453-2455.	1.0	6
116	Magnetism of close packed Fe ₁₄₇ clusters. Phase Transitions, 2006, 79, 701-707.	0.6	4
117	Possible one-dimensional structures obtained from transition metal atom doped silicon nanoclusters. Phase Transitions, 2006, 79, 709-716.	0.6	3
118	Modelling the phase diagram of magnetic shape memory Heusler alloys. Journal Physics D: Applied Physics, 2006, 39, 865-889.	1.3	306
119	Domain formation in hollow spherical Invar nano-particles. Phase Transitions, 2005, 78, 711-721.	0.6	0
120	Preparation and properties of nanostructured magnetic hollow microspheres: experiment and simulation. Phase Transitions, 2005, 78, 741-750.	0.6	21
121	Simulation of the (p,â€%T) phase diagram of the temperature-driven metamagnet $\hat{\text{I}}_{\pm}$ -FeRh. Phase Transitions, 2005, 78, 209-217.	0.6	7
122	Instability of the rhodium magnetic moment as the origin of the metamagnetic phase transition in $\hat{\text{I}}_{\pm}$ -FeRh. Physical Review B, 2003, 67, .	1.1	89
123	Modeling Structural and Magnetic Phase Transitions in Iron-Nickel Nanoparticles. Phase Transitions, 2003, 76, 355-365.	0.6	42
124	High-Moment-Low-Moment Description of Magnetovolume Effects in $\text{Y}(\text{Mn} \times \text{Al} \hat{1}^{\wedge} \times)_2$ and $\text{Y} \times \text{Sc} \hat{1}^{\wedge} \times \text{Mn} 2$. Phase Transitions, 2002, 75, 221-230.	0.6	2
125	Simulation of Magnetovolume Effects in $\text{Fe}_{65}\text{Ni}_{35}$ Nanoparticles. Progress of Theoretical Physics Supplement, 2000, 138, 154-155.	0.2	1
126	MONTE CARLO STUDY OF THE MAGNETOELASTIC PROPERTIES OF FE-NI CLUSTERS. , 2000, , .		1

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127	Monte Carlo simulations of magnetovolume instabilities in anti-Invar systems. Computational Materials Science, 1998, 10, 230-234.	1.4	2
128	Monte Carlo simulations of high-moment - low-moment transitions in Invar alloys. European Physical Journal B, 1998, 2, 107-119.	0.6	16
129	Shape Memory Alloys: A Summary of Recent Achievements. Materials Science Forum, 0, 583, 21-41.	0.3	64
130	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
131	Composition-Dependent Basics of Smart Heusler Materials from First- Principles Calculations. Materials Science Forum, 0, 684, 1-29.	0.3	39