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List of Publications by Year
in descending order

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129 papers	4,160 citations	126907 33 h-index	128289 60 g-index
132 all docs	132 docs citations	132 times ranked	5013 citing authors

#	Article	IF	Citations
1	Lattice thermal conductivity of half-Heuslers with density functional theory and machine learning: Enhancing predictivity by active sampling with principal component analysis. Computational Materials Science, 2022, 202, 110938.	3.0	17
2	Attaining Low Lattice Thermal Conductivity in Half-Heusler Sublattice Solid Solutions: Which Substitution Site Is Most Effective?. Electronic Materials, 2022, 3, 1-14.	1.9	1
3	A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+. Advanced Energy Materials, 2022, 12, .	19.5	70
4	High entropy alloy CrFeNiCoCu sputter deposited films: Structure, electrical properties, and oxidation. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2022, 40, .	2.1	3
5	New structure and insight on the phase transition within the Cu-Pd-Sn system with 25 at. % Sn. Materialia, 2022, 24, 101461.	2.7	0
6	Fabrication of a Silicide Thermoelectric Module Employing Fractional Factorial Design Principles. Journal of Electronic Materials, 2021, 50, 4041-4049.	2.2	4
7	Jahn-Teller active fluoroperovskites ACrF3 (A=Na+,K+) : Magnetic and thermo-optical properties. Physical Review Materials, 2021, 5, .	2.4	1
8	Discarded gems: Thermoelectric performance of materials with band gap emerging at the hybrid-functional level. Applied Physics Letters, 2021, 119, .	3.3	3
9	Vacancy diffusion in palladium hydrides. Physical Chemistry Chemical Physics, 2021, 23, 13680-13686.	2.8	6
10	Screening of thermoelectric silicides with atomistic transport calculations. Journal of Applied Physics, 2020, 128, 125105.	2.5	3
11	Hydrogen induced vacancy clustering and void formation mechanisms at grain boundaries in palladium. Acta Materialia, 2020, 195, 708-719.	7.9	25
12	Structural and magnetic characterization of the elusive Jahn-Teller active <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NaCrF</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review Materials, 2020, 4, .	2.4	5
13	Determining the Optimal Phase-Change Material via High-Throughput Calculations. MRS Advances, 2019, 4, 2679-2687.	0.9	4
14	A Review of Eutectic Au-Ge Solder Joints. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2019, 50, 4632-4641.	2.2	5
15	Investigation of the electrostatic potential of a grain boundary in Y-substituted BaZrO3 using inline electron holography. Physical Chemistry Chemical Physics, 2019, 21, 17662-17672.	2.8	10
16	Thermoelectric transport trends in group 4 half-Heusler alloys. Journal of Applied Physics, 2019, 126, .	2.5	20
17	Calculation of the anisotropic coefficients of thermal expansion: A first-principles approach. Computational Materials Science, 2019, 167, 257-263.	3.0	16
18	Application of machine learning-based selective sampling to determine BaZrO3 grain boundary structures. Computational Materials Science, 2019, 164, 57-65.	3.0	4

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19	Decohesion Energy of $$Sigma 5(012)$$ Grain Boundaries in Ni as Function of Hydrogen Content. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2019, 50, 451-456.	2.2	3
20	Effectiveness of Neural Networks for Research on Novel Thermoelectric Materials. A Proof of Concept. Communications in Computer and Information Science, 2019, , 69-77.	0.5	0
21	Segregation of Mg, Cu and their effects on the strength of Al Î£5 (210)[001] symmetrical tilt grain boundary. Acta Materialia, 2018, 145, 235-246.	7.9	101
22	Valence charge distribution in homogenous silicon-aluminium thin-films. Journal of Physics Condensed Matter, 2018, 30, 335502.	1.8	2
23	Optical and Microstructural Investigation of Heavy B-Doping Effects in Sublimation-Grown 3C-SiC. Materials Science Forum, 2018, 924, 221-224.	0.3	1
24	Discovering Thermoelectric Materials Using Machine Learning: Insights and Challenges. Lecture Notes in Computer Science, 2018, , 392-401.	1.3	6
25	Grain Boundary Segregation in Pd-Cu-Ag Alloys for High Permeability Hydrogen Separation Membranes. Membranes, 2018, 8, 81.	3.0	7
26	Predicting the thermoelectric figure-of-merit from first principles. Materials Today: Proceedings, 2018, 5, 10227-10234.	1.8	5
27	Formation of nanoporous Si upon self-organized growth of Al and Si nanostructures. Nanotechnology, 2018, 29, 315602.	2.6	7
28	Leakage evolution and atomic-scale changes in Pd-based membranes induced by long-term hydrogen permeation. Journal of Membrane Science, 2018, 563, 398-404.	8.2	23
29	Boron-doping of cubic SiC for intermediate band solar cells: a scanning transmission electron microscopy study. SciPost Physics, 2018, 5, .	4.9	3
30	Lattice thermal conductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ti</mml:mi><mml:mi>x</mml:mi></mml:ms alloys calculated from first principles: Key role of nature of phonon modes. Physical Review B, 2017, 95, .	3.2	79
31	Optimising multi-frame ADF-STEM for high-precision atomic-resolution strain mapping. Ultramicroscopy, 2017, 179, 57-62.	1.9	46
32	The role of grain boundary scattering in reducing the thermal conductivity of polycrystalline XNiSn (Xâ€‰=â€‰Hf, Zr, Ti) half-Heusler alloys. Scientific Reports, 2017, 7, 13760.	3.3	55
33	Characterization of B-Implanted 3C-SiC for Intermediate Band Solar Cells. Materials Science Forum, 2017, 897, 299-302.	0.3	2
34	Interface phenomena in magnetron sputtered Cu₂O/ZnO heterostructures. Journal of Physics Condensed Matter, 2017, 29, 435002.	1.8	5
35	Twinnability of Alâ€“Mg alloys: A first-principles interpretation. Transactions of Nonferrous Metals Society of China, 2017, 27, 1313-1318.	4.2	3
36	Combined effect of Mg and vacancy on the generalized planar fault energy of Al. Journal of Alloys and Compounds, 2017, 690, 841-850.	5.5	21

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37	Thermoelectric module for high temperature application. , 2017, , .		4
38	Mapping the Chemistry Within, and the Strain Around, Al-alloy Precipitates at Atomic Resolution by Multi-frame Scanning Transmission Electron Microscopy. Microscopy and Microanalysis, 2017, 23, 384-385.	0.4	0
39	Structural properties of Cu2O epitaxial films grown on c-axis single crystal ZnO by magnetron sputtering. Applied Physics Letters, 2016, 108, 152110.	3.3	10
40	Enhancement of thermoelectric properties by energy filtering: Theoretical potential and experimental reality in nanostructured ZnSb. Journal of Applied Physics, 2016, 119, .	2.5	31
41	Direct-to-indirect bandgap transitions in âŸ¨110âŸ© silicon nanowires. Journal of Applied Physics, 2016, 119, .	2.5	18
42	Impurity effect of Mg on the generalized planar fault energy of Al. Journal of Materials Science, 2016, 51, 6552-6568.	3.7	46
43	Epitaxial Strain-Induced Growth of CuO at Cu2O/ZnO Interfaces. Journal of Physical Chemistry C, 2016, 120, 23552-23558.	3.1	12
44	Comparing electrochemical performance of transition metal silicate cathodes and chevrel phase Mo6S8 in the analogous rechargeable Mg-ion battery system. Journal of Power Sources, 2016, 321, 76-86.	7.8	28
45	Boron-Implanted 3C-SiC for Intermediate Band Solar Cells. Materials Science Forum, 2016, 858, 291-294.	0.3	6
46	Nanocomposites of few-layer graphene oxide and alumina by density functional theory calculations. Journal of the European Ceramic Society, 2016, 36, 719-724.	5.7	12
47	Cubic silicon carbide as a potential photovoltaic material. Solar Energy Materials and Solar Cells, 2016, 145, 104-108.	6.2	41
48	Nanostructuring of Undoped ZnSb by Cryo-Milling. Journal of Electronic Materials, 2015, 44, 2578-2584.	2.2	17
49	Hydrogen embrittlement in nickel, visited by first principles modeling, cohesive zone simulation and nanomechanical testing. International Journal of Hydrogen Energy, 2015, 40, 16892-16900.	7.1	93
50	Multi-component solid solution and cluster hardening of Alâ€“Mnâ€“Si alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2015, 625, 153-157.	5.6	19
51	Prediction of solute diffusivity in Al assisted by first-principles molecular dynamics. Journal of Physics Condensed Matter, 2014, 26, 025403.	1.8	5
52	Perovskite to Postperovskite Transition in NaFeF₃. Inorganic Chemistry, 2014, 53, 12205-12214.	4.0	19
53	Detailed atomistic insight into the Î²â€³ phase in Alâ€“Mgâ€“Si alloys. Acta Materialia, 2014, 69, 126-134.	7.9	156
54	First-principles calculations on sulfur interacting with ternary Pdâ€“Ag-transition metal alloy membrane alloys. Journal of Membrane Science, 2014, 453, 525-531.	8.2	16

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55	Density Functional Study of the Î²â€³ Phase in Al-Mg-Si Alloys. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2014, 45, 2916-2924.	2.2	20
56	Initial stages of ITO/Si interface formation: In situ x-ray photoelectron spectroscopy measurements upon magnetron sputtering and atomistic modelling using density functional theory. Journal of Applied Physics, 2014, 115, 083705.	2.5	16
57	Removal of Phosphorus in Metallurgical Silicon by Rare Earth Elements. Metallurgical and Materials Transactions E, 2014, 1, 257-262.	0.5	1
58	Oxygen Nonstoichiometry in (Ca₂CoO₃)_{0.62}(CoO₂): A Combined Experimental and Computational Study. Journal of Physical Chemistry C, 2014, 118, 18899-18907.	3.1	24
59	X-ray photoelectron spectroscopy investigation of magnetron sputtered Mgâ€“Tiâ€“H thin films. International Journal of Hydrogen Energy, 2013, 38, 10704-10715.	7.1	21
60	Effect of Temperature on the Die Shear Strength of a Au-Sn SLID Bond. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2013, 44, 2914-2916.	2.2	23
61	High Temperature Interconnect and Die Attach Technology: Auâ€“Sn SLID Bonding. IEEE Transactions on Components, Packaging and Manufacturing Technology, 2013, 3, 904-914.	2.5	46
62	On the Complex Structural Picture of the Ionic Conductor Sr₆Ta₂O₁₁. Journal of Physical Chemistry C, 2013, 117, 9543-9549.	3.1	6
63	Effect of Transition Metal Dopants on Initial Mass Transport in the Dehydrogenation of NaAlH₄: Density Functional Theory Study. Journal of Physical Chemistry C, 2013, 117, 3-14.	3.1	19
64	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math>-Si<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>N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>(0001)/Si(111) interface: Phosphorus defects, valence b	3.2	11
65	Hydrogen induced stabilization of meta-stable Mg-Ti. Applied Physics Letters, 2012, 100, 111902.	3.3	7
66	Theoretical analysis of oxygen vacancies in layered sodium cobaltate, Na_xCoO_{2â^Î´}. Journal of Physics Condensed Matter, 2012, 24, 475505.	1.8	15
67	Interfacial Charge Transfer and Chemical Bonding in a Niâ€“LaNbO₄ Cermet for Proton-Conducting Solid-Oxide Fuel Cell Anodes. Chemistry of Materials, 2012, 24, 4152-4159.	6.7	16
68	Combined XPS and first principle study of metastable Mgâ€“Ti thin films. Surface and Interface Analysis, 2012, 44, 986-988.	1.8	6
69	Au-Sn SLID Bondingâ€”Properties and Possibilities. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2012, 43, 397-405.	2.1	73
70	Hydrogen energetics and charge transfer in the Ni/LaNbO4 interface from DFT calculations. International Journal of Hydrogen Energy, 2012, 37, 8033-8042.	7.1	6
71	Atomistic study of LaNbO4; surface properties and hydrogen adsorption. International Journal of Hydrogen Energy, 2012, 37, 6674-6685.	7.1	13
72	Crystal structure and dynamics of Mg(ND3)6Cl2. Physical Chemistry Chemical Physics, 2011, 13, 7644.	2.8	9

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73	Self-diffusion in Zn4Sb3 from first-principles molecular dynamics. Computational Materials Science, 2011, 50, 2663-2665.	3.0	11
74	Adjustment of the decomposition path for Na2LiAlH6 by TiF3 addition. International Journal of Hydrogen Energy, 2011, 36, 12279-12285.	7.1	8
75	Nanovoids in thermoelectric Î²-Zn4Sb3: A possibility for nanoengineering via Zn diffusion. Acta Materialia, 2011, 59, 5266-5275.	7.9	35
76	Nanostructuring in Î²â€Zn₄Sb₃ with variable starting Zn compositions. Physica Status Solidi (A) Applications and Materials Science, 2011, 208, 1652-1657.	1.8	25
77	XPS characterisation of in situ treated lanthanum oxide and hydroxide using tailored charge referencing and peak fitting procedures. Journal of Electron Spectroscopy and Related Phenomena, 2011, 184, 399-409.	1.7	449
78	Decomposition of lithium magnesium aluminum hydride. International Journal of Hydrogen Energy, 2011, 36, 7602-7611.	7.1	12
79	Electronic origins for sulfur interactions with palladium alloys for hydrogen-selective membranes. Journal of Membrane Science, 2011, 375, 96-103.	8.2	24
80	Experimental and theoretical study of electron density and structure factors in CoSb3. Ultramicroscopy, 2011, 111, 847-853.	1.9	11
81	Xâ€ray photoelectron spectroscopy study of MgH₂ thin films grown by reactive sputtering. Surface and Interface Analysis, 2010, 42, 1140-1143.	1.8	2
82	Characterization of thin and ultrathin transparent conducting oxide (TCO) films and TCOâ€Si interfaces with XPS, TEM and ab initio modeling. Surface and Interface Analysis, 2010, 42, 874-877.	1.8	7
83	Density functional calculations of Ti nanoclusters in the metastable Mg-Ti system. Physical Review B, 2010, 82, .	3.2	12
84	Role of the self-interaction error in studying chemisorption on graphene from first-principles. Physical Review B, 2010, 81, .	3.2	23
85	Bond analysis of phosphorus skutterudites: Elongated lanthanum electron buildup in LaFe4P12. Computational Materials Science, 2010, 47, 752-757.	3.0	8
86	Surface stability of potassium nitrate (KNO3) from density functional theory. Computational Materials Science, 2010, 50, 356-362.	3.0	6
87	Electronic structure studies of Niâ€“X (X: B, S, P) alloys using x-ray photoelectron spectroscopy, x-ray induced Auger electron spectroscopy and density functional theory calculations. Journal of Physics Condensed Matter, 2009, 21, 245503.	1.8	15
88	Viable storage of hydrogen in materials with off-board recharging using high-temperature electrolysis. International Journal of Hydrogen Energy, 2009, 34, 2679-2683.	7.1	7
89	Surfaces and Clusters of Mg(NH2)2 Studied by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2009, 113, 21648-21656.	3.1	4
90	Understanding adsorption of hydrogen atoms on graphene. Journal of Chemical Physics, 2009, 130, 054704.	3.0	303

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91	Reversed surface segregation in palladium-silver alloys due to hydrogen adsorption. Surface Science, 2008, 602, 2840-2844.	1.9	75
92	Comparison of the electronic structure of a thermoelectric skutterudite before and after adding rattlers: An electron energy loss study. Micron, 2008, 39, 685-689.	2.2	4
93	The crystal structure of LiMgAlD6 from combined neutron and synchrotron X-ray powder diffraction. Journal of Alloys and Compounds, 2008, 460, 64-68.	5.5	17
94	Thermodynamic modeling of the Naâ€“Alâ€“Tiâ€“H system and Ti dissolution in sodium alanates. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 624-636.	1.6	16
95	Experimental studies of Î±-AlD3 and Î±â€²-AlD3versus first-principles modelling of the alane isomorphs. Journal of Materials Chemistry, 2008, 18, 2361.	6.7	34
96	Density Functional Theory Study of the TiH₂ Interaction with a NaAlH₄ Cluster. Journal of Physical Chemistry C, 2008, 112, 15759-15764.	3.1	21
97	New filled P-based skutteruditesâ€”promising materials for thermoelectricity?. New Journal of Physics, 2008, 10, 053004.	2.9	8
98	Highly destabilized Mg-Ti-Ni-H system investigated by density functional theory and hydrogenography. Physical Review B, 2008, 77, .	3.2	39
99	Hydrogen interactions with the PdCu ordered B2 alloy. Journal of Alloys and Compounds, 2007, 446-447, 583-587.	5.5	55
100	NaAlH4Clusters with Two Titanium Atoms Added. Journal of Physical Chemistry C, 2007, 111, 8206-8213.	3.1	22
101	Integrated Experimentalâ^'Theoretical Investigation of the Naâ^'Liâ^'Alâ^'H System. Inorganic Chemistry, 2007, 46, 1401-1409.	4.0	16
102	The Crystal Structure and Surface Energy of NaAlH4:Â A Comparison of DFT Methodologies. Journal of Physical Chemistry B, 2006, 110, 622-630.	2.6	43
103	The crystal structure of Zr2NiD4.5. Acta Crystallographica Section B: Structural Science, 2006, 62, 972-978.	1.8	2
104	A density functional theory study of Ti-doped NaAlH4 clusters. Chemical Physics Letters, 2006, 426, 180-186.	2.6	25
105	First-principles study of alkaline-earth alanates. AIP Conference Proceedings, 2006, , .	0.4	4
106	Comparison of theoretical and experimental dielectric functions: Electron energy-loss spectroscopy and density-functional calculations on skutterudites. Physical Review B, 2006, 74, .	3.2	28
107	Stability of Ti in NaAlH4. Applied Physics Letters, 2006, 88, 161917.	3.3	32
108	Surface segregation in palladium based alloys from density-functional calculations. Surface Science, 2005, 583, 100-106.	1.9	113

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109	Crystal structure ofCa(AlH4)2predicted from density-functional band-structure calculations. Physical Review B, 2005, 71, .	3.2	58
110	Experimental and theoretical studies of plasma resonance and the electronic structure of binary skutterudites. Materials Research Society Symposia Proceedings, 2005, 886, 1.	0.1	0
111	Density functional calculations of Ti-enhancedNaAlH4. Physical Review B, 2005, 71, .	3.2	107
112	Density-functional band-structure calculations of magnesium alanateMg(AlH4)2. Physical Review B, 2005, 72, .	3.2	27
113	Modeling alkali alanates for hydrogen storage by density-functional band-structure calculations. Journal of Materials Research, 2005, 20, 3199-3213.	2.6	41
114	Crystal structures and electronic structures of alkali aluminohexahydrides from density functional calculations. Journal of Alloys and Compounds, 2005, 404-406, 757-761.	5.5	16
115	Structure and stability of possible new alanates. Europhysics Letters, 2004, 67, 607-613.	2.0	41
116	Crystal structure and thermodynamic stability of the lithium alanatesLiAlH4andLi3AlH6. Physical Review B, 2004, 69, .	3.2	114
117	The influence of electronic structure on hydrogen absorption in palladium alloys. Journal of Physics Condensed Matter, 2004, 16, 6267-6277.	1.8	75
118	Density-functional band-structure calculations for La-, Y-, and Sc-filledCoP3-based skutterudite structures. Physical Review B, 2004, 70, .	3.2	27
119	Adsorption of Ti on LiAlH4 surfaces studied by band structure calculations. Journal of Alloys and Compounds, 2004, 373, 28-32.	5.5	13
120	Density functional calculations of hydrogen adsorption on palladiumâ€“silver alloy surfaces. Journal of Chemical Physics, 2003, 118, 3268-3276.	3.0	62
121	Periodic band calculation on low index surfaces of crystalline LiAlH4. Journal of Alloys and Compounds, 2003, 356-357, 178-180.	5.5	14
122	Density functional calculations on hydrogen in palladiumâ€“silver alloys. Journal of Alloys and Compounds, 2002, 330-332, 332-337.	5.5	56
123	A study of a polymer-based radiative cooling system. Solar Energy, 2002, 73, 403-417.	6.1	97
124	Adsorption energies and ordered structures of hydrogen on Pd(111) from density-functional periodic calculations. Physical Review B, 1998, 58, 10890-10898.	3.2	81
125	The influence of surface motion on the direct subsurface absorption of H2 on Pd(111). Journal of Chemical Physics, 1997, 107, 10652-10661.	3.0	39
126	Direct subsurface absorption of hydrogen on Pd(111): Quantum mechanical calculations on a new two-dimensional potential energy surface. Journal of Chemical Physics, 1997, 106, 9286-9296.	3.0	43

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127	Direct subsurface absorption of hydrogen on Pd(111). Journal of Chemical Physics, 1996, 104, 4330-4336.	3.0	9
128	Model calculations on a flat-plate solar heat collector with integrated solar cells. Solar Energy, 1995, 55, 453-462.	6.1	290
129	Controlling the Electrical Properties of Reactively Sputtered High Entropy Alloy CrFeNiCoCu Films. Journal of Electronic Materials, 0, , 1.	2.2	1