Maximilian Amsler

List of Publications by Year
in descending order

69 papers	3,013 citations	172207 29 h-index	161609 54 g-index
72 all docs	72 docs citations	72 times ranked	3376 citing authors

#	Article	IF	Citations
1	Crystal Structure of Cold Compressed Graphite. Physical Review Letters, 2012, 108, 065501.	2.9	292
2	Crystal structure prediction using the minima hopping method. Journal of Chemical Physics, 2010, 133, 224104.	1.2	253
3	Energy Landscape of Fullerene Materials: A Comparison of Boron to Boron Nitride and Carbon. Physical Review Letters, 2011, 106, 225502.	2.9	169
4	Ultralow Thermal Conductivity in Full Heusler Semiconductors. Physical Review Letters, 2016, 117, 046602.	2.9	163
5	Low-energy silicon allotropes with strong absorption in the visible for photovoltaic applications. Physical Review B, 2012, 86, .	1.1	138
6	Achieving zT > 1 in Inexpensive Zintl Phase Ca₉Zn₄₊_xSb₉ by Phase Boundary Mapping. Advanced Functional Materials, 2017, 27, 1606361.	7.8	129
7	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. Physical Review B, 2016, 93, .	1.1	125
8	A fingerprint based metric for measuring similarities of crystalline structures. Journal of Chemical Physics, 2016, 144, 034203.	1.2	93
9	High-Pressure Structures of Disilane and Their Superconducting Properties. Physical Review Letters, 2012, 108, 117004.	2.9	86
10	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
11	Low-density silicon allotropes for photovoltaic applications. Physical Review B, 2015, 92, .	1.1	70
12	Two-Dimensional Hexagonal Sheet of TiO₂. Chemistry of Materials, 2017, 29, 8594-8603.	3.2	69
13	High accuracy and transferability of a neural network potential through charge equilibration for calcium fluoride. Physical Review B, 2017, 95, .	1.1	68
14	Unraveling the structure and bonding evolution of the newly discovered iron oxide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>FeO</mml:mi><mml:mn>2</mml:mn></mml:msub></mm Physical Review B, 2018, 98, .	1.1	62
15	Sodiumâ€“gold binaries: novel structures for ionic compounds from anab initiostructural search. New Journal of Physics, 2013, 15, 115007.	1.2	58
16	Designing and Discovering a New Family of Semiconducting Quaternary Heusler Compounds Based on the 18-Electron Rule. Chemistry of Materials, 2018, 30, 4978-4985.	3.2	57
17	Identification of Novel Cu, Ag, and Au Ternary Oxides from Global Structural Prediction. Chemistry of Materials, 2015, 27, 4562-4573.	3.2	56
18	Discovery of a Superconducting Cuâ€“Bi Intermetallic Compound by Highâ€Pressure Synthesis. Angewandte Chemie - International Edition, 2016, 55, 13446-13449.	7.2	46

#	Article	IF	Citations
19	Novel Structural Motifs in Low Energy Phases of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LiAlH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 205505.	2.9	43
20	Isomerism and Structural Fluxionality in the Au₂₆ and Au₂₆^{â€“} Nanoclusters. ACS Nano, 2014, 8, 7413-7422.	7.3	42
21	Conducting Boron Sheets Formed by the Reconstruction of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Boron (111) Surface. Physical Review Letters, 2013, 111, 136101.	2.9	40
22	Creating Binary Cuâ€“Bi Compounds via High-Pressure Synthesis: A Combined Experimental and Theoretical Study. Chemistry of Materials, 2017, 29, 5276-5285.	3.2	39
23	Low-Energy Polymeric Phases of Alanates. Physical Review Letters, 2013, 110, 135502.	2.9	38
24	Minima hopping guided path search: An efficient method for finding complex chemical reaction pathways. Journal of Chemical Physics, 2014, 140, 214102.	1.2	38
25	Crystal structure, energetics, and phase stability of strengthening precipitates in Mg alloys: A first-principles study. Acta Materialia, 2018, 158, 65-78.	3.8	35
26	Thermodynamics and superconductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi>Se</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>−</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 99, .	1.1	34
27	Carbon structures and defect planes in diamond at high pressure. Physical Review B, 2013, 88, .	1.1	32
28	Energy landscape of silicon systems and its description by force fields, tight binding schemes, density functional methods, and quantum Monte Carlo methods. Physical Review B, 2010, 81, .	1.1	31
29	First-Principles Study of Lithium Cobalt Spinel Oxides: Correlating Structure and Electrochemistry. ACS Applied Materials & Interfaces, 2018, 10, 13479-13490.	4.0	31
30	Thermodynamic stability of alkali-metalâ€“zinc double-cation borohydrides at low temperatures. Physical Review B, 2013, 88, .	1.1	29
31	Raman activity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:mrow></mml:math> allotropes under pressure: A density functional theory study. Physical Review B, 2012, 85, .	1.1	28
32	Low-energy structures of zinc borohydride Zn(BH<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 237 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	27
33	Energy landscape of ZnO clusters and low-density polymorphs. Physical Review B, 2017, 96, .	1.1	26
34	Linear scaling DFT calculations for large tungsten systems using an optimized local basis. Nuclear Materials and Energy, 2018, 15, 64-70.	0.6	26
35	Autonomous materials synthesis via hierarchical active learning of nonequilibrium phase diagrams. Science Advances, 2021, 7, eabg4930.	4.7	26
36	First-principles predicted low-energy structures of NaSc(BH4)4. Journal of Chemical Physics, 2014, 140, 124708.	1.2	25

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37	Materials Design On-the-Fly. Journal of Chemical Theory and Computation, 2015, 11, 3955-3960.	2.3	25
38	Prediction of superconducting ironâ€“bismuth intermetallic compounds at high pressure. Chemical Science, 2017, 8, 2226-2234.	3.7	25
39	FLAME: A library of atomistic modeling environments. Computer Physics Communications, 2020, 256, 107415.	3.0	23
40	Novel crystal structures for lithiumâ€“silicon alloy predicted by minima hopping method. Journal of Alloys and Compounds, 2016, 655, 147-154.	2.8	21
41	Optimized symmetry functions for machine-learning interatomic potentials of multicomponent systems. Journal of Chemical Physics, 2018, 149, 124106.	1.2	19
42	Evidence for carbon clusters present near thermal gate oxides affecting the electronic band structure in SiC-MOSFET. Applied Physics Letters, 2019, 115, .	1.5	19
43	Surfactant-assisted synthesis of large Cu-BTC MOF single crystals and their potential utilization as photodetectors. CrystEngComm, 2019, 21, 3948-3953.	1.3	19
44	Low-Energy Phases of Bi Monolayer Predicted by Structure Search in Two Dimensions. Journal of Physical Chemistry Letters, 2019, 10, 7324-7332.	2.1	18
45	ZnSb Polymorphs with Improved Thermoelectric Properties. Chemistry of Materials, 2016, 28, 2912-2920.	3.2	16
46	High-temperature conventional superconductivity in the boron-carbon system: Material trends. Physical Review B, 2020, 102, .	1.1	16
47	Ternary mixed-anion semiconductors with tunable band gaps from machine-learning and crystal structure prediction. Physical Review Materials, 2019, 3, .	0.9	16
48	Exploring the High-Pressure Materials Genome. Physical Review X, 2018, 8, .	2.8	15
49	Surface reconstruction of fluorites in vacuum and aqueous environment. Physical Review Materials, 2017, 1, .	0.9	15
50	Emergence of hidden phases of methylammonium lead iodide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>CH</mml:mi><mml:n upon compression. Physical Review Materials, 2018, 2, .	0.9	15
51	Novel phases of lithium-aluminum binaries from first-principles structural search. Journal of Chemical Physics, 2015, 142, 024710.	1.2	14
52	Discovery of a Superconducting Cuâ€“Bi Intermetallic Compound by Highâ€Pressure Synthesis. Angewandte Chemie, 2016, 128, 13644-13647.	1.6	14
53	Prediction of Superconductivity in Porous, Covalent Triazine Frameworks. , 2019, 1, 30-36.		14
54	Prediction of a novel monoclinic carbon allotrope. European Physical Journal B, 2013, 86, 1.	0.6	13

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55	The crystal structure of p-type transparent conductive oxide CuBO2. MRS Communications, 2013, 3, 157-160.	0.8	12
56	Adsorption of small NaCl clusters on surfaces of silicon nanostructures. Nanotechnology, 2009, 20, 445301.	1.3	11
57	Boron aggregation in the ground states of boron-carbon fullerenes. Physical Review B, 2014, 89, .	1.1	11
58	Cubine, a Quasi Two-Dimensional Copperâ€“Bismuth Nanosheet. Chemistry of Materials, 2017, 29, 9819-9828.	3.2	11
59	High-pressure discovery of Î²-NiBi. Chemical Communications, 2017, 53, 11241-11244.	2.2	11
60	Thermal conductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ca</mml:mi><mml:msub><mml:mi mathvariant="normal">F</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>at high pressure. Physical Review B, 2021, 103, .	1.1	7
61	Dense superconducting phases of copper-bismuth at high pressure. Physical Review Materials, 2017, 1, .	0.9	7
62	Oxygen Evolution Reaction Activity of Sr₂Ta₂O₇ and Sr₂Nb₂O₇ Surfaces. Journal of Physical Chemistry C, 2022, 126, 6556-6563.	1.5	6
63	Comment on â€œTopological Insulators in Ternary Compounds with a Honeycomb Latticeâ€• Physical Review Letters, 2013, 110, 129701.	2.9	4
64	Optical Identification of Materials Transformations in Oxide Thin Films. ACS Combinatorial Science, 2020, 22, 887-894.	3.8	4
65	Energetic and vibrational analysis of hydrogenated silicon<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>m</mml:mi></mml:math>vacancies above saturation. Physical Review B, 2014, 90, .	1.1	3
66	Comment on â€œTowards Direct-Gap Silicon Phases by the Inverse Band Structure Design Approachâ€• Physical Review Letters, 2014, 112, 199801.	2.9	2
67	Minima Hopping Method for Predicting Complex Structures and Chemical Reaction Pathways. , 2020, , 2791-2810.		2
68	Minima Hopping Method for Predicting Complex Structures and Chemical Reaction Pathways. , 2019, , 1-20.		1
69	Conformational Gap Control in CsTaS₃. Journal of the American Chemical Society, 2022, 144, 3398-3410.	6.6	1