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	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
2	Conformational Gap Control in CsTaS₃. Journal of the American Chemical Society, 2022, 144, 3398-3410.	6.6	1
3	Oxygen Evolution Reaction Activity of Sr₂Ta₂O₇ and Sr₂Nb₂O₇ Surfaces. Journal of Physical Chemistry C, 2022, 126, 6556-6563.	1.5	6
4	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
5	Autonomous materials synthesis via hierarchical active learning of nonequilibrium phase diagrams. Science Advances, 2021, 7, eabg4930.	4.7	26
6	High-temperature conventional superconductivity in the boron-carbon system: Material trends. Physical Review B, 2020, 102, .	1.1	16
7	FLAME: A library of atomistic modeling environments. Computer Physics Communications, 2020, 256, 107415.	3.0	23
8	Minima Hopping Method for Predicting Complex Structures and Chemical Reaction Pathways. , 2020, , 2791-2810.		2
9	Optical Identification of Materials Transformations in Oxide Thin Films. ACS Combinatorial Science, 2020, 22, 887-894.	3.8	4
10	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
11	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
12	Surfactant-assisted synthesis of large Cu-BTC MOF single crystals and their potential utilization as photodetectors. CrystEngComm, 2019, 21, 3948-3953.	1.3	19
13	Prediction of Superconductivity in Porous, Covalent Triazine Frameworks. , 2019, 1, 30-36.		14
14	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> mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 99, .	1.1	34
15	Minima Hopping Method for Predicting Complex Structures and Chemical Reaction Pathways. , 2019, , 1-20.		1
16	Ternary mixed-anion semiconductors with tunable band gaps from machine-learning and crystal structure prediction. Physical Review Materials, 2019, 3, .	0.9	16
17	First-Principles Study of Lithium Cobalt Spinel Oxides: Correlating Structure and Electrochemistry. ACS Applied Materials & Interfaces, 2018, 10, 13479-13490.	4.0	31
18	Linear scaling DFT calculations for large tungsten systems using an optimized local basis. Nuclear Materials and Energy, 2018, 15, 64-70.	0.6	26

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19	Exploring the High-Pressure Materials Genome. Physical Review X, 2018, 8, .	2.8	15
20	Optimized symmetry functions for machine-learning interatomic potentials of multicomponent systems. Journal of Chemical Physics, 2018, 149, 124106.	1.2	19
21	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></m Physical Review B, 2018, 98, .	1.1	62
22	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
23	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
24	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 upon compression. Physical Review Materials, 2018, 2, .	0.9	15
25	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
26	Achieving zT > 1 in Inexpensive Zintl Phase Ca₉Zn₄₊_xSb₉ by Phase Boundary Mapping. Advanced Functional Materials, 2017, 27, 1606361.	7.8	129
27	High accuracy and transferability of a neural network potential through charge equilibration for calcium fluoride. Physical Review B, 2017, 95, .	1.1	68
28	Prediction of superconducting ironâ€“bismuth intermetallic compounds at high pressure. Chemical Science, 2017, 8, 2226-2234.	3.7	25
29	Cubine, a Quasi Two-Dimensional Copperâ€“Bismuth Nanosheet. Chemistry of Materials, 2017, 29, 9819-9828.	3.2	11
30	High-pressure discovery of Î²-NiBi. Chemical Communications, 2017, 53, 11241-11244.	2.2	11
31	Two-Dimensional Hexagonal Sheet of TiO₂. Chemistry of Materials, 2017, 29, 8594-8603.	3.2	69
32	Energy landscape of ZnO clusters and low-density polymorphs. Physical Review B, 2017, 96, .	1.1	26
33	Dense superconducting phases of copper-bismuth at high pressure. Physical Review Materials, 2017, 1, .	0.9	7
34	Surface reconstruction of fluorites in vacuum and aqueous environment. Physical Review Materials, 2017, 1, .	0.9	15
35	A fingerprint based metric for measuring similarities of crystalline structures. Journal of Chemical Physics, 2016, 144, 034203.	1.2	93
36	Discovery of a Superconducting Cuâ€“Bi Intermetallic Compound by Highâ€Pressure Synthesis. Angewandte Chemie - International Edition, 2016, 55, 13446-13449.	7.2	46

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37	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. Physical Review B, 2016, 93, .	1.1	125
38	Ultralow Thermal Conductivity in Full Heusler Semiconductors. Physical Review Letters, 2016, 117, 046602.	2.9	163
39	Discovery of a Superconducting Cuâ€“Bi Intermetallic Compound by Highâ€Pressure Synthesis. Angewandte Chemie, 2016, 128, 13644-13647.	1.6	14
40	ZnSb Polymorphs with Improved Thermoelectric Properties. Chemistry of Materials, 2016, 28, 2912-2920.	3.2	16
41	Novel crystal structures for lithiumâ€“silicon alloy predicted by minima hopping method. Journal of Alloys and Compounds, 2016, 655, 147-154.	2.8	21
42	Low-density silicon allotropes for photovoltaic applications. Physical Review B, 2015, 92, .	1.1	70
43	Identification of Novel Cu, Ag, and Au Ternary Oxides from Global Structural Prediction. Chemistry of Materials, 2015, 27, 4562-4573.	3.2	56
44	Materials Design On-the-Fly. Journal of Chemical Theory and Computation, 2015, 11, 3955-3960.	2.3	25
45	Novel phases of lithium-aluminum binaries from first-principles structural search. Journal of Chemical Physics, 2015, 142, 024710.	1.2	14
46	Minima hopping guided path search: An efficient method for finding complex chemical reaction pathways. Journal of Chemical Physics, 2014, 140, 214102.	1.2	38
47	Comment on â€œTowards Direct-Gap Silicon Phases by the Inverse Band Structure Design Approachâ€. Physical Review Letters, 2014, 112, 199801.	2.9	2
48	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
49	First-principles predicted low-energy structures of NaSc(BH4)4. Journal of Chemical Physics, 2014, 140, 124708.	1.2	25
50	Boron aggregation in the ground states of boron-carbon fullerenes. Physical Review B, 2014, 89, .	1.1	11
51	Isomerism and Structural Fluxionality in the Au₂₆ and Au₂₆^{â€“} Nanoclusters. ACS Nano, 2014, 8, 7413-7422.	7.3	42
52	Carbon structures and defect planes in diamond at high pressure. Physical Review B, 2013, 88, .	1.1	32
53	Prediction of a novel monoclinic carbon allotrope. European Physical Journal B, 2013, 86, 1.	0.6	13
54	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

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55	Comment on â€œTopological Insulators in Ternary Compounds with a Honeycomb Latticeâ€• Physical Review Letters, 2013, 110, 129701.	2.9	4
56	Sodiumâ€“gold binaries: novel structures for ionic compounds from anab initiostructural search. New Journal of Physics, 2013, 15, 115007.	1.2	58
57	Thermodynamic stability of alkali-metalâ€“zinc double-cation borohydrides at low temperatures. Physical Review B, 2013, 88, .	1.1	29
58	Low-Energy Polymeric Phases of Alanates. Physical Review Letters, 2013, 110, 135502.	2.9	38
59	The crystal structure of p-type transparent conductive oxide CuBO2. MRS Communications, 2013, 3, 157-160.	0.8	12
60	Low-energy structures of zinc borohydride Zn(BH<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 557 Td (xmlns:mml="http://www.w3 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
61	Low-energy silicon allotropes with strong absorption in the visible for photovoltaic applications. Physical Review B, 2012, 86, .	1.1	138
62	High-Pressure Structures of Disilane and Their Superconducting Properties. Physical Review Letters, 2012, 108, 117004.	2.9	86
63	Raman activity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:m allotropes under pressure: A density functional theory study. Physical Review B, 2012, 85, .	1.1	28
64	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
65	Crystal Structure of Cold Compressed Graphite. Physical Review Letters, 2012, 108, 065501.	2.9	292
66	Energy Landscape of Fullerene Materials: A Comparison of Boron to Boron Nitride and Carbon. Physical Review Letters, 2011, 106, 225502.	2.9	169
67	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
68	Crystal structure prediction using the minima hopping method. Journal of Chemical Physics, 2010, 133, 224104.	1.2	253
69	Adsorption of small NaCl clusters on surfaces of silicon nanostructures. Nanotechnology, 2009, 20, 445301.	1.3	11