Maximilian Amsler

List of Publications by Citations

68 papers	2,327 citations	26 h-index	47 g-index
72 ext. papers	2,712 ext. citations	5.8 avg, IF	5.17 L-index

#	Paper	IF	Citations
68	Crystal structure of cold compressed graphite. *Physical Review Letters*, **2012**, 108, 065501	7.4	265
67	Crystal structure prediction using the minima hopping method. *Journal of Chemical Physics*, **2010**, 133, 224104	3.9	215
66	Energy landscape of fullerene materials: a comparison of boron to boron nitride and carbon. *Physical Review Letters*, **2011**, 106, 225502	7.4	152
65	Low-energy silicon allotropes with strong absorption in the visible for photovoltaic applications. *Physical Review B*, **2012**, 86,	3.3	116
64	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. *Physical Review B*, **2016**, 93,	3.3	108
63	Ultralow Thermal Conductivity in Full Heusler Semiconductors. *Physical Review Letters*, **2016**, 117, 046602	7.4	103
62	Achieving zT > 1 in Inexpensive Zintl Phase Ca9Zn4+xSb9 by Phase Boundary Mapping. *Advanced Functional Materials*, **2017**, 27, 1606361	15.6	98
61	High-pressure structures of disilane and their superconducting properties. *Physical Review Letters*, **2012**, 108, 117004	7.4	80
60	A fingerprint based metric for measuring similarities of crystalline structures. *Journal of Chemical Physics*, **2016**, 144, 034203	3.9	75
59	Low-density silicon allotropes for photovoltaic applications. *Physical Review B*, **2015**, 92,	3.3	58
58	Unraveling the structure and bonding evolution of the newly discovered iron oxide FeO2. *Physical Review B*, **2018**, 98,	3.3	51
57	Two-Dimensional Hexagonal Sheet of TiO2. *Chemistry of Materials*, **2017**, 29, 8594-8603	9.6	51
56	High accuracy and transferability of a neural network potential through charge equilibration for calcium fluoride. *Physical Review B*, **2017**, 95,	3.3	48
55	Identification of Novel Cu, Ag, and Au Ternary Oxides from Global Structural Prediction. *Chemistry of Materials*, **2015**, 27, 4562-4573	9.6	47
54	Novel structural motifs in low energy phases of LiAlH4. *Physical Review Letters*, **2012**, 108, 205505	7.4	42
53	Isomerism and structural fluxionality in the Au26 and Au26(-) nanoclusters. *ACS Nano*, **2014**, 8, 7413-22	16.7	40
52	Conducting boron sheets formed by the reconstruction of the □boron (111) surface. *Physical Review Letters*, **2013**, 111, 136101	7.4	39

51	Discovery of a Superconducting Cu-Bi Intermetallic Compound by High-Pressure Synthesis. *Angewandte Chemie - International Edition*, **2016**, 55, 13446-13449	16.4	37
50	Sodium□gold binaries: novel structures for ionic compounds from anab initiostructural search. *New Journal of Physics*, **2013**, 15, 115007	2.9	36
49	Creating Binary Cu□Bi Compounds via High-Pressure Synthesis: A Combined Experimental and Theoretical Study. *Chemistry of Materials*, **2017**, 29, 5276-5285	9.6	34
48	Low-energy polymeric phases of alanates. *Physical Review Letters*, **2013**, 110, 135502	7.4	33
47	Minima hopping guided path search: an efficient method for finding complex chemical reaction pathways. *Journal of Chemical Physics*, **2014**, 140, 214102	3.9	32
46	Carbon structures and defect planes in diamond at high pressure. *Physical Review B*, **2013**, 88,	3.3	30
45	Thermodynamic stability of alkali-metal□inc double-cation borohydrides at low temperatures. *Physical Review B*, **2013**, 88,	3.3	27
44	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,	3.3	27
43	Designing and Discovering a New Family of Semiconducting Quaternary Heusler Compounds Based on the 18-Electron Rule. *Chemistry of Materials*, **2018**, 30, 4978-4985	9.6	26
42	Low-energy structures of zinc borohydride Zn(BH4)2. *Physical Review B*, **2012**, 86,	3.3	26
41	Raman activity of sp3 carbon allotropes under pressure: A density functional theory study. *Physical Review B*, **2012**, 85,	3.3	25
40	Materials Design On-the-Fly. *Journal of Chemical Theory and Computation*, **2015**, 11, 3955-60	6.4	24
39	Prediction of superconducting iron-bismuth intermetallic compounds at high pressure. *Chemical Science*, **2017**, 8, 2226-2234	9.4	20
38	Thermodynamics and superconductivity of SxSe1□H3. *Physical Review B*, **2019**, 99,	3.3	20
37	Crystal structure, energetics, and phase stability of strengthening precipitates in Mg alloys: A first-principles study. *Acta Materialia*, **2018**, 158, 65-78	8.4	20
36	First-Principles Study of Lithium Cobalt Spinel Oxides: Correlating Structure and Electrochemistry. *ACS Applied Materials & Interfaces*, **2018**, 10, 13479-13490	9.5	19
35	Linear scaling DFT calculations for large tungsten systems using an optimized local basis. *Nuclear Materials and Energy*, **2018**, 15, 64-70	2.1	19
34	Energy landscape of ZnO clusters and low-density polymorphs. *Physical Review B*, **2017**, 96,	3.3	18

33	Novel crystal structures for lithium silicon alloy predicted by minima hopping method. *Journal of Alloys and Compounds*, **2016**, 655, 147-154	5.7	17
32	First-principles predicted low-energy structures of NaSc(BH4)4. *Journal of Chemical Physics*, **2014**, 140, 124708	3.9	17
31	FLAME: A library of atomistic modeling environments. *Computer Physics Communications*, **2020**, 256, 107415	4.2	13
30	ZnSb Polymorphs with Improved Thermoelectric Properties. *Chemistry of Materials*, **2016**, 28, 2912-2920	9.6	13
29	Prediction of a novel monoclinic carbon allotrope. *European Physical Journal B*, **2013**, 86, 1	1.2	13
28	Surface reconstruction of fluorites in vacuum and aqueous environment. *Physical Review Materials*, **2017**, 1,	3.2	13
27	Novel phases of lithium-aluminum binaries from first-principles structural search. *Journal of Chemical Physics*, **2015**, 142, 024710	3.9	12
26	Discovery of a Superconducting CuBi Intermetallic Compound by High-Pressure Synthesis. *Angewandte Chemie*, **2016**, 128, 13644-13647	3.6	11
25	Adsorption of small NaCl clusters on surfaces of silicon nanostructures. *Nanotechnology*, **2009**, 20, 445301	3.4	11
24	Optimized symmetry functions for machine-learning interatomic potentials of multicomponent systems. *Journal of Chemical Physics*, **2018**, 149, 124106	3.9	11
23	Cubine, a Quasi Two-Dimensional CopperBismuth Nanosheet. *Chemistry of Materials*, **2017**, 29, 9819-9828	9.6	10
22	Evidence for carbon clusters present near thermal gate oxides affecting the electronic band structure in SiC-MOSFET. *Applied Physics Letters*, **2019**, 115, 101601	3.4	10
21	Prediction of Superconductivity in Porous, Covalent Triazine Frameworks **2019**, 1, 30-36		10
20	High-pressure discovery of NiBi. *Chemical Communications*, **2017**, 53, 11241-11244	5.8	10
19	The crystal structure of p-type transparent conductive oxide CuBO2. *MRS Communications*, **2013**, 3, 157-160	1.7	10
18	Boron aggregation in the ground states of boron-carbon fullerenes. *Physical Review B*, **2014**, 89,	3.3	9
17	Exploring the High-Pressure Materials Genome. *Physical Review X*, **2018**, 8,	9.1	9
16	The 2021 Room-Temperature Superconductivity Roadmap. *Journal of Physics Condensed Matter*, **2021**,	1.8	9

List of Publications

15	Surfactant-assisted synthesis of large Cu-BTC MOF single crystals and their potential utilization as photodetectors. *CrystEngComm*, **2019**, 21, 3948-3953	3.3	8
14	Low-Energy Phases of Bi Monolayer Predicted by Structure Search in Two Dimensions. *Journal of Physical Chemistry Letters*, **2019**, 10, 7324-7332	6.4	8
13	Emergence of hidden phases of methylammonium lead iodide (CH3NH3PbI3) upon compression. *Physical Review Materials*, **2018**, 2,	3.2	7
12	Dense superconducting phases of copper-bismuth at high pressure. *Physical Review Materials*, **2017**, 1,	3.2	6
11	Ternary mixed-anion semiconductors with tunable band gaps from machine-learning and crystal structure prediction. *Physical Review Materials*, **2019**, 3,	3.2	5
10	Comment on "Topological insulators in ternary compounds with a honeycomb lattice". *Physical Review Letters*, **2013**, 110, 129701	7.4	4
9	High-temperature conventional superconductivity in the boron-carbon system: Material trends. *Physical Review B*, **2020**, 102,	3.3	4
8	Energetic and vibrational analysis of hydrogenated silicon m vacancies above saturation. *Physical Review B*, **2014**, 90,	3.3	3
7	Optical Identification of Materials Transformations in Oxide Thin Films. *ACS Combinatorial Science*, **2020**, 22, 887-894	3.9	3
6	Autonomous materials synthesis via hierarchical active learning of nonequilibrium phase diagrams.. *Science Advances*, **2021**, 7, eabg4930	14.3	3
5	Comment on "Towards direct-gap silicon phases by the inverse band structure design approach". *Physical Review Letters*, **2014**, 112, 199801	7.4	2
4	Thermal conductivity of CaF2 at high pressure. *Physical Review B*, **2021**, 103,	3.3	2
3	Minima Hopping Method for Predicting Complex Structures and Chemical Reaction Pathways **2020**, 2791-2810		1
2	Minima Hopping Method for Predicting Complex Structures and Chemical Reaction Pathways **2019**, 1-20		1
1	Oxygen Evolution Reaction Activity of Sr2Ta2O7 and Sr2Nb2O7 Surfaces. *Journal of Physical Chemistry C*, **2022**, 126, 6556-6563	3.8	1