Volker L Deringer

List of Publications by Citations

109 papers	6,725 citations	36 h-index	81 g-index
122 ext. papers	8,820 ext. citations	8.8 avg, IF	6.76 L-index

#	Paper	IF	Citations
109	Crystal orbital Hamilton population (COHP) analysis as projected from plane-wave basis sets. *Journal of Physical Chemistry A*, **2011**, 115, 5461-6	2.8	1057
108	Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. *Journal of Computational Chemistry*, **2013**, 34, 2557-67	3.5	790
107	Machine learning based interatomic potential for amorphous carbon. *Physical Review B*, **2017**, 95,	3.3	293
106	A stable compound of helium and sodium at high pressure. *Nature Chemistry*, **2017**, 9, 440-445	17.6	199
105	Machine Learning Interatomic Potentials as Emerging Tools for Materials Science. *Advanced Materials*, **2019**, 31, e1902765	24	177
104	LOBSTER: Local orbital projections, atomic charges, and chemical-bonding analysis from projector-augmented-wave-based density-functional theory. *Journal of Computational Chemistry*, **2020**, 41, 1931-1940	3.5	155
103	Incipient Metals: Functional Materials with a Unique Bonding Mechanism. *Advanced Materials*, **2018**, 30, e1803777	24	154
102	A Quantum-Mechanical Map for Bonding and Properties in Solids. *Advanced Materials*, **2019**, 31, e1806280	24	134
101	Realistic Atomistic Structure of Amorphous Silicon from Machine-Learning-Driven Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2018**, 9, 2879-2885	6.4	114
100	Data-Driven Learning of Total and Local Energies in Elemental Boron. *Physical Review Letters*, **2018**, 120, 156001	7.4	112
99	Bonding nature of local structural motifs in amorphous GeTe. *Angewandte Chemie - International Edition*, **2014**, 53, 10817-20	16.4	102
98	Cooperativity of halogen, chalcogen, and pnictogen bonds in infinite molecular chains by electronic structure theory. *Journal of Physical Chemistry A*, **2014**, 118, 3193-200	2.8	81
97	Growth Mechanism and Origin of High sp^{3} Content in Tetrahedral Amorphous Carbon. *Physical Review Letters*, **2018**, 120, 166101	7.4	80
96	De novo exploration and self-guided learning of potential-energy surfaces. *Npj Computational Materials*, **2019**, 5,	10.9	73
95	Microscopic Complexity in Phase-Change Materials and its Role for Applications. *Advanced Functional Materials*, **2015**, 25, 6343-6359	15.6	71
94	Accurate Hydrogen Positions in Organic Crystals: Assessing a Quantum-Chemical Aide. *Crystal Growth and Design*, **2012**, 12, 1014-1021	3.5	66
93	Origins of structural and electronic transitions in disordered silicon. *Nature*, **2021**, 589, 59-64	50.4	66

92	Gaussian Process Regression for Materials and Molecules. *Chemical Reviews*, **2021**, 121, 10073-10141	68.1	66
91	Extracting Crystal Chemistry from Amorphous Carbon Structures. *ChemPhysChem*, **2017**, 18, 873-877	3.2	63
90	Vibrational properties and bonding nature of SbSe and their implications for chalcogenide materials. *Chemical Science*, **2015**, 6, 5255-5262	9.4	62
89	Modeling the Phase-Change Memory Material, GeSbTe, with a Machine-Learned Interatomic Potential. *Journal of Physical Chemistry B*, **2018**, 122, 8998-9006	3.4	62
88	Towards an atomistic understanding of disordered carbon electrode materials. *Chemical Communications*, **2018**, 54, 5988-5991	5.8	56
87	Density-functional theory guided advances in phase-change materials and memories. *MRS Bulletin*, **2015**, 40, 856-869	3.2	52
86	Gaussian approximation potential modeling of lithium intercalation in carbon nanostructures. *Journal of Chemical Physics*, **2018**, 148, 241714	3.9	50
85	An accurate and transferable machine learning potential for carbon. *Journal of Chemical Physics*, **2020**, 153, 034702	3.9	49
84	Reactivity of Amorphous Carbon Surfaces: Rationalizing the Role of Structural Motifs in Functionalization Using Machine Learning. *Chemistry of Materials*, **2018**, 30, 7446-7455	9.6	49
83	Similarity Between Amorphous and Crystalline Phases: The Case of TiO. *Journal of Physical Chemistry Letters*, **2018**, 9, 2985-2990	6.4	49
82	Vibrational and thermodynamic properties of GeSe in the quasiharmonic approximation. *Physical Review B*, **2014**, 89,	3.3	48
81	Ab Initio Modeling of GeTe(111) Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 15801-15811	3.8	48
80	Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory. *Chemistry of Materials*, **2018**, 30, 7438-7445	9.6	48
79	Understanding the thermal properties of amorphous solids using machine-learning-based interatomic potentials. *Molecular Simulation*, **2018**, 44, 866-880	2	47
78	Plane-Wave Density Functional Theory Meets Molecular Crystals: Thermal Ellipsoids and Intermolecular Interactions. *Accounts of Chemical Research*, **2017**, 50, 1231-1239	24.3	41
77	Data-driven learning and prediction of inorganic crystal structures. *Faraday Discussions*, **2018**, 211, 45-59	3.6	40
76	Covalency of hydrogen bonds in solids revisited. *Chemical Communications*, **2014**, 50, 11547-9	5.8	39
75	Nature, Strength, and Cooperativity of the Hydrogen-Bonding Network in Chitin. *Biomacromolecules*, **2016**, 17, 996-1003	6.9	39

74	First-principles study of alkali-metal intercalation in disordered carbon anode materials. *Journal of Materials Chemistry A*, **2019**, 7, 19070-19080	13	35
73	A chemical link between Ge–Sb–Te and In–Sb–Te phase-change materials. *Journal of Materials Chemistry C*, **2015**, 3, 9519-9523	7.1	34
72	Understanding X-ray Spectroscopy of Carbonaceous Materials by Combining Experiments, Density Functional Theory, and Machine Learning. Part I: Fingerprint Spectra. *Chemistry of Materials*, **2019**, 31, 9243-9255	9.6	33
71	Chemical Design Principles for Cache-Type Sc–Sb–Te Phase-Change Memory Materials. *Chemistry of Materials*, **2019**, 31, 4008-4015	9.6	32
70	Fast Ionic Conductivity in the Most Lithium-Rich Phosphidosilicate LiSiP. *Journal of the American Chemical Society*, **2019**, 141, 14200-14209	16.4	32
69	Mechanisms of Atomic Motion Through Crystalline GeTe. *Chemistry of Materials*, **2013**, 25, 2220-2226	9.6	30
68	Thermochemical Ranking and Dynamic Stability of TeO2 Polymorphs from Ab Initio Theory. *Crystal Growth and Design*, **2014**, 14, 871-878	3.5	29
67	Hydrogen-bonding networks from first-principles: exploring the guanidine crystal. *Journal of Physical Chemistry A*, **2012**, 116, 4551-9	2.8	29
66	Ab initio ORTEP drawings: a case study of N-based molecular crystals with different chemical nature. *CrystEngComm*, **2014**, 16, 10907-10915	3.3	28
65	A general-purpose machine-learning force field for bulk and nanostructured phosphorus. *Nature Communications*, **2020**, 11, 5461	17.4	28
64	Anisotropic displacement parameters from dispersion-corrected DFT methods and their experimental validation by temperature-dependent X-ray diffraction. *CrystEngComm*, **2015**, 17, 7414-7422	3.3	27
63	DFT Studies of Pristine Hexagonal Ge1Sb2Te4(0001), Ge2Sb2Te5(0001), and Ge1Sb4Te7(0001) Surfaces. *Journal of Physical Chemistry C*, **2013**, 117, 15075-15089	3.8	27
62	Mapping Materials and Molecules. *Accounts of Chemical Research*, **2020**, 53, 1981-1991	24.3	27
61	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. *Angewandte Chemie - International Edition*, **2019**, 58, 7057-7061	16.4	26
60	Understanding X-ray Spectroscopy of Carbonaceous Materials by Combining Experiments, Density Functional Theory, and Machine Learning. Part II: Quantitative Fitting of Spectra. *Chemistry of Materials*, **2019**, 31, 9256-9267	9.6	26
59	Modelling and understanding battery materials with machine-learning-driven atomistic simulations. *JPhys Energy*, **2020**, 2, 041003	4.9	25
58	Stability of pristine and defective SnTe surfaces from first principles. *ChemPhysChem*, **2013**, 14, 3108-11	3.2	23
57	Chemical understanding of resistance drift suppression in Ge–Sn–Te phase-change memory materials. *Journal of Materials Chemistry C*, **2020**, 8, 71-77	7.1	22

56	Bonding similarities and differences between Y$_2$Sb$_3$Te and Sc$_2$Sb$_3$Te phase-change memory materials. *Journal of Materials Chemistry C*, **2020**, 8, 3646-3654	7.1	21
55	Unconventional two-dimensional germanium dichalcogenides. *Nanoscale*, **2018**, 10, 7363-7368	7.7	21
54	Machine learning driven simulated deposition of carbon films: From low-density to diamondlike amorphous carbon. *Physical Review B*, **2020**, 102,	3.3	20
53	From Atomistic Surface Chemistry to Nanocrystals of Functional Chalcogenides. *Angewandte Chemie - International Edition*, **2015**, 54, 15334-40	16.4	19
52	Dimensionality of intermolecular interactions in layered crystals by electronic-structure theory and geometric analysis. *Inorganic Chemistry*, **2015**, 54, 956-62	5.1	18
51	A density-functional study on the electronic and vibrational properties of layered antimony telluride. *Journal of Physics Condensed Matter*, **2015**, 27, 085402	1.8	18
50	Ab initio molecular dynamics and materials design for embedded phase-change memory. *Npj Computational Materials*, **2021**, 7,	10.9	18
49	High-pressure synthesis and characterization of Li2Ca3[N2]3--an uncommon metallic diazenide with [N2]2- ions. *Journal of the American Chemical Society*, **2013**, 135, 16668-79	16.4	17
48	Chemical Tuning of Carrier Type and Concentration in a Homologous Series of Crystalline Chalcogenides. *Chemistry of Materials*, **2017**, 29, 6749-6757	9.6	17
47	Lattice thermal expansion and anisotropic displacements in ?-sulfur from diffraction experiments and first-principles theory. *Journal of Chemical Physics*, **2016**, 145, 234512	3.9	17
46	Exploring Chemical Bonding in Phase-Change Materials with Orbital-Based Indicators. *Physica Status Solidi - Rapid Research Letters*, **2019**, 13, 1800579	2.5	16
45	Pauling's third rule beyond the bulk: chemical bonding at quartz-type GeO2 surfaces. *Chemical Science*, **2014**, 5, 894-903	9.4	16
44	Intermolecular contacts in bromomalonic aldehyde: intuition, experiment, and theory. *CrystEngComm*, **2014**, 16, 135-138	3.3	16
43	Fast Lithium Ion Conduction in Lithium Phosphidoaluminates. *Angewandte Chemie - International Edition*, **2020**, 59, 5665-5674	16.4	16
42	Hierarchically Structured Allotropes of Phosphorus from Data-Driven Exploration. *Angewandte Chemie - International Edition*, **2020**, 59, 15880-15885	16.4	15
41	Completing a family: LiCN3H4, the lightest alkali metal guanidinate. *Dalton Transactions*, **2013**, 42, 15080-3	4.5	15
40	Stabilities and Reconstructions of PbTe Crystal Surfaces from Density-Functional Theory. *Journal of Physical Chemistry C*, **2013**, 117, 24455-24461	3.8	15
39	On the DFT ground state of crystalline bromine and iodine. *ChemPhysChem*, **2015**, 16, 728-32	3.2	14

38	Anisotropic thermal motion in transition-metal carbonyls from experiments and ab initio theory. *Dalton Transactions*, **2016**, 45, 13680-5	4.3	14
37	Chemical modeling of mixed occupations and site preferences in anisotropic crystal structures: case of complex intermetallic borides. *Inorganic Chemistry*, **2012**, 51, 5677-85	5.1	14
36	Synthesis, crystal structure, chemical bonding, and physical properties of the ternary Na/Mg stannide Na2MgSn. *Inorganic Chemistry*, **2012**, 51, 4810-6	5.1	14
35	Structural and elastic properties of amorphous carbon from simulated quenching at low rates. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 085009	2	14
34	Orbital mixing in solids as a descriptor for materials mapping. *Solid State Communications*, **2015**, 203, 31-34	1.6	13
33	Sub-Angstrom Characterization of the Structural Origin for High In-Plane Anisotropy in 2D GeS. *ACS Nano*, **2020**, 14, 4456-4462	16.7	13
32	Understanding the Shape of GeTe Nanocrystals from First Principles. *Chemistry of Materials*, **2016**, 28, 6682-6688	9.6	13
31	Ab initio study of the high-temperature phase transition in crystalline GeO2. *Journal of Computational Chemistry*, **2013**, 34, 2320-6	3.5	13
30	Combining phonon accuracy with high transferability in Gaussian approximation potential models. *Journal of Chemical Physics*, **2020**, 153, 044104	3.9	13
29	Ab initio lattice dynamics and thermochemistry of layered bismuth telluride (Bi2Te3). *Journal of Physics Condensed Matter*, **2016**, 28, 115401	1.8	13
28	Stabilities and Reconstructions of Clean PbS and PbSe Surfaces: DFT Results and the Role of Dispersion Forces. *Journal of Physical Chemistry C*, **2016**, 120, 8813-8820	3.8	13
27	Materials Screening for Disorder-Controlled Chalcogenide Crystals for Phase-Change Memory Applications. *Advanced Materials*, **2021**, 33, e2006221	24	13
26	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. *Angewandte Chemie*, **2019**, 131, 7131-7135	3.6	12
25	Many-Body Dispersion Correction Effects on Bulk and Surface Properties of Rutile and Anatase TiO2. *Journal of Physical Chemistry C*, **2016**, 120, 21552-21560	3.8	10
24	Ab initio study of molecular and atomic oxygen on GeTe(111) surfaces. *Journal of Applied Physics*, **2014**, 116, 173703	2.5	10
23	Understanding the geometric diversity of inorganic and hybrid frameworks through structural coarse-graining. *Chemical Science*, **2020**, 11, 12580-12587	9.4	9
22	Synthesis, crystal structure, and high-temperature phase transition of the novel plumbide Na2MgPb. *Inorganic Chemistry*, **2014**, 53, 5253-9	5.1	7
21	Exploring the subsurface atomic structure of the epitaxially grown phase-change material Ge2Sb2Te5. *Physical Review B*, **2017**, 96,	3.3	7

20	A transferable active-learning strategy for reactive molecular force fields. *Chemical Science*, **2021**, 12, 10944-10955	9.4	7
19	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. *Faraday Discussions*, **2018**, 211, 325-381	3.6	6
18	Neutron powder diffraction and theory-aided structure refinement of rubidium and cesium ureate. *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **2016**, 71, 431-438	1	5
17	Visualization and Quantification of Geometric Diversity in Metal□Organic Frameworks. *Chemistry of Materials*,	9.6	5
16	Fast Lithium Ion Conduction in Lithium Phosphidoaluminates. *Angewandte Chemie*, **2020**, 132, 5714-5723	3.6	5
15	Bindungseigenschaften lokaler Strukturmotive in amorphem GeTe. *Angewandte Chemie*, **2014**, 126, 10993-10997	3.6	5
14	Structure and Dynamics of Supercooled Liquid Ge2Sb2Te5 from Machine-Learning-Driven Simulations. *Physica Status Solidi - Rapid Research Letters*, **2021**, 15, 2000403	2.5	3
13	Supertetrahedral polyanionic network in the first lithium phosphidoindate LiInP - structural similarity to LiSiP and LiGeP and dissimilarity to LiAlP and LiGaP. *Chemical Science*, **2020**, 12, 1278-1285	9.4	3
12	Structure searching methods: general discussion. *Faraday Discussions*, **2018**, 211, 133-180	3.6	3
11	Unraveling Crystallization Mechanisms and Electronic Structure of Phase-Change Materials by Large-Scale Ab Initio Simulations.. *Advanced Materials*, **2022**, e2109139	24	2
10	X-ray Spectroscopy Fingerprints of Pristine and Functionalized Graphene. *Journal of Physical Chemistry C*, **2021**, 125, 18234-18246	3.8	2
9	Bonding nature and optical contrast of TiTe2/Sb2Te3 phase-change heterostructure. *Materials Science in Semiconductor Processing*, **2021**, 135, 106080	4.3	2
8	Hierarchically Structured Allotropes of Phosphorus from Data-Driven Exploration. *Angewandte Chemie*, **2020**, 132, 16014-16019	3.6	1
7	Ge□Sb□Te Phase-Change Materials **2017**, 735-749		1
6	Von atomistischer Oberfl□chenchemie zu Nanokristallen funktionaler Chalkogenide. *Angewandte Chemie*, **2015**, 127, 15550-15557	3.6	1
5	Phonon Spectroscopy in Antimony and Tellurium Oxides. *Journal of Physical Chemistry A*, **2020**, 124, 7869-7880	2.8	1
4	Cluster Fragments in Amorphous Phosphorus and their Evolution under Pressure. *Advanced Materials*, **2021**, e2107515	24	0
3	Unraveling Crystallization Mechanisms and Electronic Structure of Phase-Change Materials by Large-Scale Ab Initio Simulations (Adv. Mater. 11/2022). *Advanced Materials*, **2022**, 34, 2270084	24	0

2 Nanosession: Phase Change Memories **2013**, 163-176

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