

Volker L Deringer

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Unraveling Crystallization Mechanisms and Electronic Structure of Phase-Change Materials by Large-Scale Ab Initio Simulations.. <i>Advanced Materials</i> , 2022 , e2109139	24	2
108	Unraveling Crystallization Mechanisms and Electronic Structure of Phase-Change Materials by Large-Scale Ab Initio Simulations (Adv. Mater. 11/2022). <i>Advanced Materials</i> , 2022 , 34, 2270084	24	0
107	Cluster Fragments in Amorphous Phosphorus and their Evolution under Pressure. <i>Advanced Materials</i> , 2021 , e2107515	24	0
106	Structure and Dynamics of Supercooled Liquid Ge ₂ Sb ₂ Te ₅ from Machine-Learning-Driven Simulations. <i>Physica Status Solidi - Rapid Research Letters</i> , 2021 , 15, 2000403	2.5	3
105	Origins of structural and electronic transitions in disordered silicon. <i>Nature</i> , 2021 , 589, 59-64	50.4	66
104	Ab initio molecular dynamics and materials design for embedded phase-change memory. <i>Npj Computational Materials</i> , 2021 , 7,	10.9	18
103	X-ray Spectroscopy Fingerprints of Pristine and Functionalized Graphene. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 18234-18246	3.8	2
102	Gaussian Process Regression for Materials and Molecules. <i>Chemical Reviews</i> , 2021 , 121, 10073-10141	68.1	66
101	Bonding nature and optical contrast of TiTe ₂ /Sb ₂ Te ₃ phase-change heterostructure. <i>Materials Science in Semiconductor Processing</i> , 2021 , 135, 106080	4.3	2
100	Materials Screening for Disorder-Controlled Chalcogenide Crystals for Phase-Change Memory Applications. <i>Advanced Materials</i> , 2021 , 33, e2006221	24	13
99	A transferable active-learning strategy for reactive molecular force fields. <i>Chemical Science</i> , 2021 , 12, 10944-10955	9.4	7
98	Hierarchically Structured Allotropes of Phosphorus from Data-Driven Exploration. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 15880-15885	16.4	15
97	Hierarchically Structured Allotropes of Phosphorus from Data-Driven Exploration. <i>Angewandte Chemie</i> , 2020 , 132, 16014-16019	3.6	1
96	LOBSTER: Local orbital projections, atomic charges, and chemical-bonding analysis from projector-augmented-wave-based density-functional theory. <i>Journal of Computational Chemistry</i> , 2020 , 41, 1931-1940	3.5	155
95	Bonding similarities and differences between Yb ₂ Te and Sc ₂ Te phase-change memory materials. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 3646-3654	7.1	21
94	Sub-Angstrom Characterization of the Structural Origin for High In-Plane Anisotropy in 2D GeS. <i>ACS Nano</i> , 2020 , 14, 4456-4462	16.7	13
93	Modelling and understanding battery materials with machine-learning-driven atomistic simulations. <i>JPhys Energy</i> , 2020 , 2, 041003	4.9	25

92	Chemical understanding of resistance drift suppression in GeSbTe phase-change memory materials. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 71-77	7.1	22
91	Fast Lithium Ion Conduction in Lithium Phosphidoaluminates. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 5665-5674	16.4	16
90	Fast Lithium Ion Conduction in Lithium Phosphidoaluminates. <i>Angewandte Chemie</i> , 2020 , 132, 5714-5723	3.6	5
89	Understanding the geometric diversity of inorganic and hybrid frameworks through structural coarse-graining. <i>Chemical Science</i> , 2020 , 11, 12580-12587	9.4	9
88	Combining phonon accuracy with high transferability in Gaussian approximation potential models. <i>Journal of Chemical Physics</i> , 2020 , 153, 044104	3.9	13
87	An accurate and transferable machine learning potential for carbon. <i>Journal of Chemical Physics</i> , 2020 , 153, 034702	3.9	49
86	Mapping Materials and Molecules. <i>Accounts of Chemical Research</i> , 2020 , 53, 1981-1991	24.3	27
85	Machine learning driven simulated deposition of carbon films: From low-density to diamondlike amorphous carbon. <i>Physical Review B</i> , 2020 , 102,	3.3	20
84	A general-purpose machine-learning force field for bulk and nanostructured phosphorus. <i>Nature Communications</i> , 2020 , 11, 5461	17.4	28
83	Phonon Spectroscopy in Antimony and Tellurium Oxides. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 7869-7880	2.8	1
82	Supertetrahedral polyanionic network in the first lithium phosphidoindate LiInP - structural similarity to LiSiP and LiGeP and dissimilarity to LiAlP and LiGaP. <i>Chemical Science</i> , 2020 , 12, 1278-1285	9.4	3
81	Exploring Chemical Bonding in Phase-Change Materials with Orbital-Based Indicators. <i>Physica Status Solidi - Rapid Research Letters</i> , 2019 , 13, 1800579	2.5	16
80	Chemical Design Principles for Cache-Type ScSbTe Phase-Change Memory Materials. <i>Chemistry of Materials</i> , 2019 , 31, 4008-4015	9.6	32
79	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 7057-7061	16.4	26
78	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. <i>Angewandte Chemie</i> , 2019 , 131, 7131-7135	3.6	12
77	Fast Ionic Conductivity in the Most Lithium-Rich Phosphidosilicate LiSiP. <i>Journal of the American Chemical Society</i> , 2019 , 141, 14200-14209	16.4	32
76	First-principles study of alkali-metal intercalation in disordered carbon anode materials. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 19070-19080	13	35
75	Machine Learning Interatomic Potentials as Emerging Tools for Materials Science. <i>Advanced Materials</i> , 2019 , 31, e1902765	24	177

74	De novo exploration and self-guided learning of potential-energy surfaces. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	73
73	Understanding X-ray Spectroscopy of Carbonaceous Materials by Combining Experiments, Density Functional Theory, and Machine Learning. Part II: Quantitative Fitting of Spectra. <i>Chemistry of Materials</i> , 2019 , 31, 9256-9267	9.6	26
72	Understanding X-ray Spectroscopy of Carbonaceous Materials by Combining Experiments, Density Functional Theory, and Machine Learning. Part I: Fingerprint Spectra. <i>Chemistry of Materials</i> , 2019 , 31, 9243-9255	9.6	33
71	Structural and elastic properties of amorphous carbon from simulated quenching at low rates. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019 , 27, 085009	2	14
70	A Quantum-Mechanical Map for Bonding and Properties in Solids. <i>Advanced Materials</i> , 2019 , 31, e1806280	10.4	134
69	Growth Mechanism and Origin of High sp^3 Content in Tetrahedral Amorphous Carbon. <i>Physical Review Letters</i> , 2018 , 120, 166101	7.4	80
68	Gaussian approximation potential modeling of lithium intercalation in carbon nanostructures. <i>Journal of Chemical Physics</i> , 2018 , 148, 241714	3.9	50
67	Data-Driven Learning of Total and Local Energies in Elemental Boron. <i>Physical Review Letters</i> , 2018 , 120, 156001	7.4	112
66	Data-driven learning and prediction of inorganic crystal structures. <i>Faraday Discussions</i> , 2018 , 211, 45-59	3.6	40
65	Understanding the thermal properties of amorphous solids using machine-learning-based interatomic potentials. <i>Molecular Simulation</i> , 2018 , 44, 866-880	2	47
64	Unconventional two-dimensional germanium dichalcogenides. <i>Nanoscale</i> , 2018 , 10, 7363-7368	7.7	21
63	Structure searching methods: general discussion. <i>Faraday Discussions</i> , 2018 , 211, 133-180	3.6	3
62	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. <i>Faraday Discussions</i> , 2018 , 211, 325-381	3.6	6
61	Incipient Metals: Functional Materials with a Unique Bonding Mechanism. <i>Advanced Materials</i> , 2018 , 30, e1803777	24	154
60	Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory. <i>Chemistry of Materials</i> , 2018 , 30, 7438-7445	9.6	48
59	Reactivity of Amorphous Carbon Surfaces: Rationalizing the Role of Structural Motifs in Functionalization Using Machine Learning. <i>Chemistry of Materials</i> , 2018 , 30, 7446-7455	9.6	49
58	Modeling the Phase-Change Memory Material, GeSbTe, with a Machine-Learned Interatomic Potential. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 8998-9006	3.4	62
57	Towards an atomistic understanding of disordered carbon electrode materials. <i>Chemical Communications</i> , 2018 , 54, 5988-5991	5.8	56

56	Realistic Atomistic Structure of Amorphous Silicon from Machine-Learning-Driven Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 2879-2885	6.4	114
55	Similarity Between Amorphous and Crystalline Phases: The Case of TiO. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 2985-2990	6.4	49
54	Extracting Crystal Chemistry from Amorphous Carbon Structures. <i>ChemPhysChem</i> , 2017 , 18, 873-877	3.2	63
53	A stable compound of helium and sodium at high pressure. <i>Nature Chemistry</i> , 2017 , 9, 440-445	17.6	199
52	Machine learning based interatomic potential for amorphous carbon. <i>Physical Review B</i> , 2017 , 95,	3.3	293
51	Plane-Wave Density Functional Theory Meets Molecular Crystals: Thermal Ellipsoids and Intermolecular Interactions. <i>Accounts of Chemical Research</i> , 2017 , 50, 1231-1239	24.3	41
50	Chemical Tuning of Carrier Type and Concentration in a Homologous Series of Crystalline Chalcogenides. <i>Chemistry of Materials</i> , 2017 , 29, 6749-6757	9.6	17
49	Exploring the subsurface atomic structure of the epitaxially grown phase-change material Ge ₂ Sb ₂ Te ₅ . <i>Physical Review B</i> , 2017 , 96,	3.3	7
48	GeSbTe Phase-Change Materials 2017 , 735-749		1
47	Understanding the Shape of GeTe Nanocrystals from First Principles. <i>Chemistry of Materials</i> , 2016 , 28, 6682-6688	9.6	13
46	Anisotropic thermal motion in transition-metal carbonyls from experiments and ab initio theory. <i>Dalton Transactions</i> , 2016 , 45, 13680-5	4.3	14
45	Many-Body Dispersion Correction Effects on Bulk and Surface Properties of Rutile and Anatase TiO ₂ . <i>Journal of Physical Chemistry C</i> , 2016 , 120, 21552-21560	3.8	10
44	Neutron powder diffraction and theory-aided structure refinement of rubidium and cesium ureate. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2016 , 71, 431-438	1	5
43	Ab initio lattice dynamics and thermochemistry of layered bismuth telluride (Bi ₂ Te ₃). <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 115401	1.8	13
42	Lattice thermal expansion and anisotropic displacements in α -sulfur from diffraction experiments and first-principles theory. <i>Journal of Chemical Physics</i> , 2016 , 145, 234512	3.9	17
41	Nature, Strength, and Cooperativity of the Hydrogen-Bonding Network in β -Chitin. <i>Biomacromolecules</i> , 2016 , 17, 996-1003	6.9	39
40	Stabilities and Reconstructions of Clean PbS and PbSe Surfaces: DFT Results and the Role of Dispersion Forces. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 8813-8820	3.8	13
39	On the DFT ground state of crystalline bromine and iodine. <i>ChemPhysChem</i> , 2015 , 16, 728-32	3.2	14

38	Vibrational properties and bonding nature of SbSe and their implications for chalcogenide materials. <i>Chemical Science</i> , 2015 , 6, 5255-5262	9.4	62
37	Anisotropic displacement parameters from dispersion-corrected DFT methods and their experimental validation by temperature-dependent X-ray diffraction. <i>CrystEngComm</i> , 2015 , 17, 7414-7422	3.3	27
36	A chemical link between GeSbTe and InSbTe phase-change materials. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 9519-9523	7.1	34
35	Orbital mixing in solids as a descriptor for materials mapping. <i>Solid State Communications</i> , 2015 , 203, 31-34	1.6	13
34	Dimensionality of intermolecular interactions in layered crystals by electronic-structure theory and geometric analysis. <i>Inorganic Chemistry</i> , 2015 , 54, 956-62	5.1	18
33	Density-functional theory guided advances in phase-change materials and memories. <i>MRS Bulletin</i> , 2015 , 40, 856-869	3.2	52
32	From Atomistic Surface Chemistry to Nanocrystals of Functional Chalcogenides. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 15334-40	16.4	19
31	Microscopic Complexity in Phase-Change Materials and its Role for Applications. <i>Advanced Functional Materials</i> , 2015 , 25, 6343-6359	15.6	71
30	Von atomistischer Oberflächenchemie zu Nanokristallen funktionaler Chalkogenide. <i>Angewandte Chemie</i> , 2015 , 127, 15550-15557	3.6	1
29	A density-functional study on the electronic and vibrational properties of layered antimony telluride. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 085402	1.8	18
28	Synthesis, crystal structure, and high-temperature phase transition of the novel plumbide Na ₂ MgPb. <i>Inorganic Chemistry</i> , 2014 , 53, 5253-9	5.1	7
27	Thermochemical Ranking and Dynamic Stability of TeO ₂ Polymorphs from Ab Initio Theory. <i>Crystal Growth and Design</i> , 2014 , 14, 871-878	3.5	29
26	Ab initio study of molecular and atomic oxygen on GeTe(111) surfaces. <i>Journal of Applied Physics</i> , 2014 , 116, 173703	2.5	10
25	Ab initio ORTEP drawings: a case study of N-based molecular crystals with different chemical nature. <i>CrystEngComm</i> , 2014 , 16, 10907-10915	3.3	28
24	Pauling's third rule beyond the bulk: chemical bonding at quartz-type GeO ₂ surfaces. <i>Chemical Science</i> , 2014 , 5, 894-903	9.4	16
23	Intermolecular contacts in bromomalonic aldehyde: intuition, experiment, and theory. <i>CrystEngComm</i> , 2014 , 16, 135-138	3.3	16
22	Covalency of hydrogen bonds in solids revisited. <i>Chemical Communications</i> , 2014 , 50, 11547-9	5.8	39
21	Vibrational and thermodynamic properties of GeSe in the quasiharmonic approximation. <i>Physical Review B</i> , 2014 , 89,	3.3	48

20	Cooperativity of halogen, chalcogen, and pnictogen bonds in infinite molecular chains by electronic structure theory. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 3193-200	2.8	81
19	Bonding nature of local structural motifs in amorphous GeTe. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 10817-20	16.4	102
18	Bindungseigenschaften lokaler Struktur motive in amorphem GeTe. <i>Angewandte Chemie</i> , 2014 , 126, 10993-10997	3.3	10997
17	Completing a family: LiCN3H4, the lightest alkali metal guanidinate. <i>Dalton Transactions</i> , 2013 , 42, 15080-7	4.3	15
16	High-pressure synthesis and characterization of Li2Ca3[N2]3--an uncommon metallic diazenide with [N2]2- ions. <i>Journal of the American Chemical Society</i> , 2013 , 135, 16668-79	16.4	17
15	Stabilities and Reconstructions of PbTe Crystal Surfaces from Density-Functional Theory. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 24455-24461	3.8	15
14	Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. <i>Journal of Computational Chemistry</i> , 2013 , 34, 2557-67	3.5	790
13	Ab initio study of the high-temperature phase transition in crystalline GeO2. <i>Journal of Computational Chemistry</i> , 2013 , 34, 2320-6	3.5	13
12	Mechanisms of Atomic Motion Through Crystalline GeTe. <i>Chemistry of Materials</i> , 2013 , 25, 2220-2226	9.6	30
11	DFT Studies of Pristine Hexagonal Ge1Sb2Te4(0001), Ge2Sb2Te5(0001), and Ge1Sb4Te7(0001) Surfaces. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 15075-15089	3.8	27
10	Stability of pristine and defective SnTe surfaces from first principles. <i>ChemPhysChem</i> , 2013 , 14, 3108-11	3.2	23
9	Nanosession: Phase Change Memories 2013 , 163-176		
8	Chemical modeling of mixed occupations and site preferences in anisotropic crystal structures: case of complex intermetallic borides. <i>Inorganic Chemistry</i> , 2012 , 51, 5677-85	5.1	14
7	Synthesis, crystal structure, chemical bonding, and physical properties of the ternary Na/Mg stannide Na2MgSn. <i>Inorganic Chemistry</i> , 2012 , 51, 4810-6	5.1	14
6	Ab Initio Modeling of β -GeTe(111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 15801-15811	3.8	48
5	Hydrogen-bonding networks from first-principles: exploring the guanidine crystal. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 4551-9	2.8	29
4	Accurate Hydrogen Positions in Organic Crystals: Assessing a Quantum-Chemical Aide. <i>Crystal Growth and Design</i> , 2012 , 12, 1014-1021	3.5	66
3	Crystal orbital Hamilton population (COHP) analysis as projected from plane-wave basis sets. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 5461-6	2.8	1057

2	Visualization and Quantification of Geometric Diversity in Metal-Organic Frameworks. <i>Chemistry of Materials</i> ,	9.6	5
1	Nanosession: Phase Change Materials	155-162	