Volker L Deringer

List of Publications by Year
in descending order

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108	11,359	61945 43	29127 104
papers	citations	h-index	g-index

122	122	122	8659
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Crystal Orbital Hamilton Population (COHP) Analysis As Projected from Plane-Wave Basis Sets. Journal of Physical Chemistry A, 2011, 115, 5461-5466.	1.1	1,823
2	LOBSTER: A tool to extract chemical bonding from planeâ€wave based DFT. Journal of Computational Chemistry, 2016, 37, 1030-1035.	1.5	1,791
3	Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. Journal of Computational Chemistry, 2013, 34, 2557-2567.	1.5	1,178
4	<scp>LOBSTER</scp>: Local orbital projections, atomic charges, and chemicalâ€bonding analysis from <scp>projectorâ€augmentedâ€waveâ€based</scp> densityâ€functional theory. Journal of Computational Chemistry, 2020, 41, 1931-1940.	1.5	523
5	Machine learning based interatomic potential for amorphous carbon. Physical Review B, 2017, 95, .	1.1	431
6	Machine Learning Interatomic Potentials as Emerging Tools for Materials Science. Advanced Materials, 2019, 31, e1902765.	11.1	389
7	Gaussian Process Regression for Materials and Molecules. Chemical Reviews, 2021, 121, 10073-10141.	23.0	384
8	A stable compound of helium and sodium at high pressure. Nature Chemistry, 2017, 9, 440-445.	6.6	276
9	Incipient Metals: Functional Materials with a Unique Bonding Mechanism. Advanced Materials, 2018, 30, e1803777.	11.1	255
10	A Quantumâ€Mechanical Map for Bonding and Properties in Solids. Advanced Materials, 2019, 31, e1806280.	11.1	206
11	Origins of structural and electronic transitions in disordered silicon. Nature, 2021, 589, 59-64.	13.7	192
12	Realistic Atomistic Structure of Amorphous Silicon from Machine-Learning-Driven Molecular Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 2879-2885.	2.1	170
13	Data-Driven Learning of Total and Local Energies in Elemental Boron. Physical Review Letters, 2018, 120, 156001.	2.9	150
14	An accurate and transferable machine learning potential for carbon. Journal of Chemical Physics, 2020, 153, 034702.	1.2	137
15	De novo exploration and self-guided learning of potential-energy surfaces. Npj Computational Materials, 2019, 5, .	3.5	132
16	Growth Mechanism and Origin of High <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:math> Content in Tetrahedral Amorphous Carbon. Physical Review Letters, 2018, 120, 166101.	2.9	128
17	Bonding Nature of Local Structural Motifs in Amorphous GeTe. Angewandte Chemie - International Edition, 2014, 53, 10817-10820.	7.2	125
18	Modeling the Phase-Change Memory Material, Ge₂Sb₂Te₅, with a Machine-Learned Interatomic Potential. Journal of Physical Chemistry B, 2018, 122, 8998-9006.	1.2	102

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19	Cooperativity of Halogen, Chalcogen, and Pnictogen Bonds in Infinite Molecular Chains by Electronic Structure Theory. Journal of Physical Chemistry A, 2014, 118, 3193-3200.	1.1	90
20	Vibrational properties and bonding nature of Sb₂Se₃and their implications for chalcogenide materials. Chemical Science, 2015, 6, 5255-5262.	3.7	89
21	Towards an atomistic understanding of disordered carbon electrode materials. Chemical Communications, 2018, 54, 5988-5991.	2.2	84
22	Extracting Crystal Chemistry from Amorphous Carbon Structures. ChemPhysChem, 2017, 18, 873-877.	1.0	80
23	Microscopic Complexity in Phaseâ€Change Materials and its Role for Applications. Advanced Functional Materials, 2015, 25, 6343-6359.	7.8	78
24	Similarity Between Amorphous and CrystallineÂPhases: TheÂCaseÂofÂTiO₂. Journal of Physical Chemistry Letters, 2018, 9, 2985-2990.	2.1	78
25	Reactivity of Amorphous Carbon Surfaces: Rationalizing the Role of Structural Motifs in Functionalization Using Machine Learning. Chemistry of Materials, 2018, 30, 7446-7455.	3.2	77
26	A general-purpose machine-learning force field for bulk and nanostructured phosphorus. Nature Communications, 2020, 11, 5461.	5.8	72
27	Gaussian approximation potential modeling of lithium intercalation in carbon nanostructures. Journal of Chemical Physics, 2018, 148, 241714.	1.2	71
28	Mapping Materials and Molecules. Accounts of Chemical Research, 2020, 53, 1981-1991.	7.6	71
29	Understanding the thermal properties of amorphous solids using machine-learning-based interatomic potentials. Molecular Simulation, 2018, 44, 866-880.	0.9	69
30	Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory. Chemistry of Materials, 2018, 30, 7438-7445.	3.2	69
31	Accurate Hydrogen Positions in Organic Crystals: Assessing a Quantum-Chemical Aide. Crystal Growth and Design, 2012, 12, 1014-1021.	1.4	68
32	First-principles study of alkali-metal intercalation in disordered carbon anode materials. Journal of Materials Chemistry A, 2019, 7, 19070-19080.	5.2	68
33	Data-driven learning and prediction of inorganic crystal structures. Faraday Discussions, 2018, 211, 45-59.	1.6	66
34	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.	3.2	62
35	Vibrational and thermodynamic properties of GeSe in the quasiharmonic approximation. Physical Review B, 2014, 89, .	1.1	59
36	Density-functional theory guided advances in phase-change materials and memories. MRS Bulletin, 2015, 40, 856-869.	1.7	57

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37	Nature, Strength, and Cooperativity of the Hydrogen-Bonding Network in Î±-Chitin. Biomacromolecules, 2016, 17, 996-1003.	2.6	57
38	Ab Initio Modeling of Î±-GeTe(111) Surfaces. Journal of Physical Chemistry C, 2012, 116, 15801-15811.	1.5	55
39	Modelling and understanding battery materials with machine-learning-driven atomistic simulations. JPhys Energy, 2020, 2, 041003.	2.3	51
40	Covalency of hydrogen bonds in solids revisited. Chemical Communications, 2014, 50, 11547-11549.	2.2	50
41	Fast Ionic Conductivity in the Most Lithium-Rich Phosphidosilicate Li₁₄SiP₆. Journal of the American Chemical Society, 2019, 141, 14200-14209.	6.6	49
42	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.	3.2	49
43	Plane-Wave Density Functional Theory Meets Molecular Crystals: Thermal Ellipsoids and Intermolecular Interactions. Accounts of Chemical Research, 2017, 50, 1231-1239.	7.6	47
44	A chemical link between Geâ€“Sbâ€“Te and Inâ€“Sbâ€“Te phase-change materials. Journal of Materials Chemistry C, 2015, 3, 9519-9523.	2.7	44
45	Chemical Design Principles for Cache-Type Scâ€“Sbâ€“Te Phase-Change Memory Materials. Chemistry of Materials, 2019, 31, 4008-4015.	3.2	44
46	Machine learning driven simulated deposition of carbon films: From low-density to diamondlike amorphous carbon. Physical Review B, 2020, 102, .	1.1	44
47	Ab initio molecular dynamics and materials design for embedded phase-change memory. Npj Computational Materials, 2021, 7, .	3.5	44
48	Mechanisms of Atomic Motion Through Crystalline GeTe. Chemistry of Materials, 2013, 25, 2220-2226.	3.2	38
49	Chemical understanding of resistance drift suppression in Geâ€“Snâ€“Te phase-change memory materials. Journal of Materials Chemistry C, 2020, 8, 71-77.	2.7	36
50	A machine-learned interatomic potential for silica and its relation to empirical models. Npj Computational Materials, 2022, 8, .	3.5	36
51	Quantifying Chemical Structure and Machineâ€Learned Atomic Energies in Amorphous and Liquid Silicon. Angewandte Chemie - International Edition, 2019, 58, 7057-7061.	7.2	35
52	Thermochemical Ranking and Dynamic Stability of TeO₂ Polymorphs from Ab Initio Theory. Crystal Growth and Design, 2014, 14, 871-878.	1.4	32
53	Ab initio ORTEP drawings: a case study of N-based molecular crystals with different chemical nature. CrystEngComm, 2014, 16, 10907-10915.	1.3	32
54	Materials Screening for Disorderâ€Controlled Chalcogenide Crystals for Phaseâ€Change Memory Applications. Advanced Materials, 2021, 33, e2006221.	11.1	32

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55	Hydrogen-Bonding Networks from First-Principles: Exploring the Guanidine Crystal. Journal of Physical Chemistry A, 2012, 116, 4551-4559.	1.1	31
56	Structural and elastic properties of amorphous carbon from simulated quenching at low rates. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 085009.	0.8	30
57	DFT Studies of Pristine Hexagonal Ge₁Sb₂Te₄(0001), Ge₂Sb₂Te₅(0001), and Ge₁Sb₄Te₇(0001) Surfaces. Journal of Physical Chemistry C, 2013, 117, 15075-15089.	1.5	29
58	Combining phonon accuracy with high transferability in Gaussian approximation potential models. Journal of Chemical Physics, 2020, 153, 044104.	1.2	29
59	Fast Lithium Ion Conduction in Lithium Phosphidoaluminates. Angewandte Chemie - International Edition, 2020, 59, 5665-5674.	7.2	28
60	Bonding similarities and differences between Yâ€“Sbâ€“Te and Scâ€“Sbâ€“Te phase-change memory materials. Journal of Materials Chemistry C, 2020, 8, 3646-3654.	2.7	28
61	Anisotropic displacement parameters from dispersion-corrected DFT methods and their experimental validation by temperature-dependent X-ray diffraction. CrystEngComm, 2015, 17, 7414-7422.	1.3	27
62	Stability of Pristine and Defective SnTe Surfaces from First Principles. ChemPhysChem, 2013, 14, 3108-3111.	1.0	26
63	Unconventional two-dimensional germanium dichalcogenides. Nanoscale, 2018, 10, 7363-7368.	2.8	26
64	Hierarchically Structured Allotropes of Phosphorus from Dataâ€Driven Exploration. Angewandte Chemie - International Edition, 2020, 59, 15880-15885.	7.2	26
65	A transferable active-learning strategy for reactive molecular force fields. Chemical Science, 2021, 12, 10944-10955.	3.7	26
66	Sub-Angstrom Characterization of the Structural Origin for High In-Plane Anisotropy in 2D GeS₂. ACS Nano, 2020, 14, 4456-4462.	7.3	25
67	Exploring Chemical Bonding in Phaseâ€Change Materials with Orbitalâ€Based Indicators. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800579.	1.2	22
68	Unraveling Crystallization Mechanisms and Electronic Structure of Phaseâ€Change Materials by Largeâ€Scale Ab Initio Simulations. Advanced Materials, 2022, 34, e2109139.	11.1	21
69	Stabilities and Reconstructions of PbTe Crystal Surfaces from Density-Functional Theory. Journal of Physical Chemistry C, 2013, 117, 24455-24461.	1.5	20
70	From Atomistic Surface Chemistry to Nanocrystals of Functional Chalcogenides. Angewandte Chemie - International Edition, 2015, 54, 15334-15340.	7.2	20
71	On the DFT Ground State of Crystalline Bromine and Iodine. ChemPhysChem, 2015, 16, 728-732.	1.0	20
72	Synthesis, Crystal Structure, Chemical Bonding, and Physical Properties of the Ternary Na/Mg Stannide Na₂MgSn. Inorganic Chemistry, 2012, 51, 4810-4816.	1.9	19

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73	High-Pressure Synthesis and Characterization of Li₂Ca₃[N₂]₃â€”An Uncommon Metallic Diazenide with [N₂]^{2â€“} Ions. Journal of the American Chemical Society, 2013, 135, 16668-16679.	6.6	19
74	Lattice thermal expansion and anisotropic displacements in ?-sulfur from diffraction experiments and first-principles theory. Journal of Chemical Physics, 2016, 145, 234512.	1.2	19
75	A density-functional study on the electronic and vibrational properties of layered antimony telluride. Journal of Physics Condensed Matter, 2015, 27, 085402.	0.7	18
76	Dimensionality of Intermolecular Interactions in Layered Crystals by Electronic-Structure Theory and Geometric Analysis. Inorganic Chemistry, 2015, 54, 956-962.	1.9	18
77	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.	1.5	18
78	Chemical Tuning of Carrier Type and Concentration in a Homologous Series of Crystalline Chalcogenides. Chemistry of Materials, 2017, 29, 6749-6757.	3.2	18
79	Quantifying Chemical Structure and Machineâ€Learned Atomic Energies in Amorphous and Liquid Silicon. Angewandte Chemie, 2019, 131, 7131-7135.	1.6	18
80	Chemical Modeling of Mixed Occupations and Site Preferences in Anisotropic Crystal Structures: Case of Complex Intermetallic Borides. Inorganic Chemistry, 2012, 51, 5677-5685.	1.9	17
81	Completing a family: LiCN3H4, the lightest alkali metal guanidinate. Dalton Transactions, 2013, 42, 15080.	1.6	17
82	Pauling's third rule beyond the bulk: chemical bonding at quartz-type GeO2surfaces. Chemical Science, 2014, 5, 894-903.	3.7	17
83	Intermolecular contacts in bromomalonic aldehydeâ€”intuition, experiment, and theory. CrystEngComm, 2014, 16, 135-138.	1.3	17
84	Ab initiolattice dynamics and thermochemistry of layered bismuth telluride (Bi₂Te₃). Journal of Physics Condensed Matter, 2016, 28, 115401.	0.7	17
85	Ab initio study of the highâ€temperature phase transition in crystalline GeO₂. Journal of Computational Chemistry, 2013, 34, 2320-2326.	1.5	16
86	Orbital mixing in solids as a descriptor for materials mapping. Solid State Communications, 2015, 203, 31-34.	0.9	16
87	Understanding the Shape of GeTe Nanocrystals from First Principles. Chemistry of Materials, 2016, 28, 6682-6688.	3.2	16
88	Anisotropic thermal motion in transition-metal carbonyls from experiments and ab initio theory. Dalton Transactions, 2016, 45, 13680-13685.	1.6	15
89	Understanding the geometric diversity of inorganic and hybrid frameworks through structural coarse-graining. Chemical Science, 2020, 11, 12580-12587.	3.7	13
90	Bonding nature and optical contrast of TiTe2/Sb2Te3 phase-change heterostructure. Materials Science in Semiconductor Processing, 2021, 135, 106080.	1.9	13

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91	Cluster Fragments in Amorphous Phosphorus and their Evolution under Pressure. Advanced Materials, 2022, 34, e2107515.	11.1	13
92	Synthesis, Crystal Structure, and High-Temperature Phase Transition of the Novel Plumbide Na2MgPb. Inorganic Chemistry, 2014, 53, 5253-5259.	1.9	11
93	Many-Body Dispersion Correction Effects on Bulk and Surface Properties of Rutile and Anatase TiO₂. Journal of Physical Chemistry C, 2016, 120, 21552-21560.	1.5	11
94	Visualization and Quantification of Geometric Diversity in Metalâ€“Organic Frameworks. Chemistry of Materials, 0, , .	3.2	11
95	Ab initio study of molecular and atomic oxygen on GeTe(111) surfaces. Journal of Applied Physics, 2014, 116, .	1.1	10
96	Exploring the subsurface atomic structure of the epitaxially grown phase-change material <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Ge</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Sb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Te</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2017, 96, .	1.1	10
97	Fast Lithium Ion Conduction in Lithium Phosphidoaluminates. Angewandte Chemie, 2020, 132, 5714-5723.	1.6	10
98	X-ray Spectroscopy Fingerprints of Pristine and Functionalized Graphene. Journal of Physical Chemistry C, 2021, 125, 18234-18246.	1.5	9
99	Supertetrahedral polyanionic network in the first lithium phosphidoindate Li₃InP₂ â€“ structural similarity to Li₂SiP₂ and Li₂GeP₂ and dissimilarity to Li₃AlP₂ and Li₃GaP₂. Chemical Science, 2021, 12, 1278-1285.	3.7	8
100	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	1.6	7
101	Phonon Spectroscopy in Antimony and Tellurium Oxides. Journal of Physical Chemistry A, 2020, 124, 7869-7880.	1.1	6
102	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.	0.3	5
103	Structure and Dynamics of Supercooled Liquid Ge₂Sb₂Te₅ from Machineâ€Learningâ€Driven Simulations. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2000403.	1.2	4
104	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	1.6	3
105	Hierarchically Structured Allotropes of Phosphorus from Dataâ€Driven Exploration. Angewandte Chemie, 2020, 132, 16014-16019.	1.6	1
106	Unraveling Crystallization Mechanisms and Electronic Structure of Phaseâ€Change Materials by Largeâ€Scale Ab Initio Simulations (Adv. Mater. 11/2022). Advanced Materials, 2022, 34, .	11.1	1
107	Frontispiece: Fast Lithium Ion Conduction in Lithium Phosphidoaluminates. Angewandte Chemie - International Edition, 2020, 59, .	7.2	0
108	Frontispiz: Fast Lithium Ion Conduction in Lithium Phosphidoaluminates. Angewandte Chemie, 2020, 132, .	1.6	0