Volker Blum

List of Publications by Year
in descending order

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114	12,233	41344	25787
papers	citations	49	108
		h-index	g-index

120	120	120	12325
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ab initio molecular simulations with numeric atom-centered orbitals. Computer Physics Communications, 2009, 180, 2175-2196.	7.5	2,170
2	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
3	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589
4	Rational design of carbon nitride photocatalysts by identification of cyanamide defects as catalytically relevant sites. Nature Communications, 2016, 7, 12165.	12.8	586
5	Resolution-of-identity approach to Hartreeâ€“Fock, hybrid density functionals, RPA, MP2 andGWwith numeric atom-centered orbital basis functions. New Journal of Physics, 2012, 14, 053020.	2.9	549
6	Efficient integration for all-electron electronic structure calculation using numeric basis functions. Journal of Computational Physics, 2009, 228, 8367-8379.	3.8	454
7	Low-Molecular-Weight Carbon Nitrides for Solar Hydrogen Evolution. Journal of the American Chemical Society, 2015, 137, 1064-1072.	13.7	321
8	Molecular engineering of organicâ€“inorganic hybrid perovskites quantum wells. Nature Chemistry, 2019, 11, 1151-1157.	13.6	302
9	Evolutionary approach for determining first-principles hamiltonians. Nature Materials, 2005, 4, 391-394.	27.5	285
10	Ureaâ€Modified Carbon Nitrides: Enhancing Photocatalytic Hydrogen Evolution by Rational Defect Engineering. Advanced Energy Materials, 2017, 7, 1602251.	19.5	238
11	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
12	The Pd()â€“R27Â°-O surface oxide revisited. Surface Science, 2003, 541, 101-112.	1.9	201
13	Organic-to-inorganic structural chirality transfer in a 2D hybrid perovskite and impact on Rashba-Dresselhaus spin-orbit coupling. Nature Communications, 2020, 11, 4699.	12.8	200
14	Highly Distorted Chiral Two-Dimensional Tin Iodide Perovskites for Spin Polarized Charge Transport. Journal of the American Chemical Society, 2020, 142, 13030-13040.	13.7	198
15	Direct and cost-efficient hyperpolarization of long-lived nuclear spin states on universal ¹⁵ N ₂ -diazirine molecular tags. Science Advances, 2016, 2, e1501438.	10.3	193
16	The ELPA library: scalable parallel eigenvalue solutions for electronic structure theory and computational science. Journal of Physics Condensed Matter, 2014, 26, 213201.	1.8	173
17	Direct-Bandgap 2D Silverâ€“Bismuth Iodide Double Perovskite: The Structure-Directing Influence of an Oligothiophene Spacer Cation. Journal of the American Chemical Society, 2019, 141, 7955-7964.	13.7	151
18	Parallel solution of partial symmetric eigenvalue problems from electronic structure calculations. Parallel Computing, 2011, 37, 783-794.	2.1	147

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19	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. Computer Physics Communications, 2015, 192, 60-69.	7.5	133
20	BaCu₂Sn(S,Se)₄: Earth-Abundant Chalcogenides for Thin-Film Photovoltaics. Chemistry of Materials, 2016, 28, 4771-4780.	6.7	131
21	Using genetic algorithms to map first-principles results to model Hamiltonians: Application to the generalized Ising model for alloys. Physical Review B, 2005, 72, .	3.2	130
22	Trapping lead in perovskite solar modules with abundant and low-cost cation-exchange resins. Nature Energy, 2020, 5, 1003-1011.	39.5	126
23	Fast LEED intensity calculations for surface crystallography using Tensor LEED. Computer Physics Communications, 2001, 134, 392-425.	7.5	119
24	Earthâ€Abundant Chalcogenide Photovoltaic Devices with over 5% Efficiency Based on a Cu₂BaSn(S,Se)₄ Absorber. Advanced Materials, 2017, 29, 1606945.	21.0	112
25	Isomer-Selective Detection of Hydrogen-Bond Vibrations in the Protonated Water Hexamer. Journal of the American Chemical Society, 2013, 135, 8266-8273.	13.7	107
26	Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites. Physical Review Letters, 2018, 121, 146401.	7.8	103
27	Unraveling the Stability of Polypeptide Helices: Critical Role of van der Waals Interactions. Physical Review Letters, 2011, 106, 118102.	7.8	97
28	Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. New Journal of Physics, 2015, 17, 093020.	2.9	97
29	The surface oxide: A LEED, DFT and STM study. Surface Science, 2007, 601, 1574-1581.	1.9	96
30	Mixed-basis cluster expansion for thermodynamics of bcc alloys. Physical Review B, 2004, 70, .	3.2	95
31	All-electron formalism for total energy strain derivatives and stress tensor components for numeric atom-centered orbitals. Computer Physics Communications, 2015, 190, 33-50.	7.5	92
32	One-hundred-three compound band-structure benchmark of post-self-consistent spin-orbit coupling treatments in density functional theory. Physical Review Materials, 2017, 1, .	2.4	92
33	The Elephant in the Room of Density Functional Theory Calculations. Journal of Physical Chemistry Letters, 2017, 8, 1449-1457.	4.6	88
34	I₂â€“IIâ€“IVâ€“VI₄ (I = Cu, Ag; II = Sr, Ba; IV = Ge, Sn; VI = S, Se): Chalcogenides for Thin-Film Photovoltaics. Chemistry of Materials, 2017, 29, 7868-7879.	6.7	87
35	Accuracy of first-principles lateral interactions: Oxygen at Pd(100). Physical Review B, 2007, 75, .	3.2	83
36	First-Principles Molecular Structure Search with a Genetic Algorithm. Journal of Chemical Information and Modeling, 2015, 55, 2338-2348.	5.4	83

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37	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. New Journal of Physics, 2013, 15, 123033.	2.9	81
38	ELSI: A unified software interface for Kohnâ€“Sham electronic structure solvers. Computer Physics Communications, 2018, 222, 267-285.	7.5	78
39	Structural descriptor for enhanced spin-splitting in 2D hybrid perovskites. Nature Communications, 2021, 12, 4982.	12.8	78
40	Secondary Structure of Ac-Ala_n-LysH⁺ Polyalanine Peptides (n =) Tj ETQq0 0 0 rgBT /Overlock 10	4.6	76
41	Approaching Truly Freestanding Graphene: The Structure of Hydrogen-Intercalated Graphene on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mn>6</mml:mn><mml:mi>H</mml:mi></mml:mrow><mml:mtext>â</mml:mtext><mml:mrow><mml:mo mathvariant="bold">(</mml:mo><mml:mn>0001</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 567 Td (mathvariant="bold">)	7.5	74
42	Prediction of unusual stable ordered structures of Au-Pd alloys via a first-principles cluster expansion. Physical Review B, 2006, 74, .	3.2	71
43	Long-Lived ¹³C₂ Nuclear Spin States Hyperpolarized by Parahydrogen in Reversible Exchange at Microtesla Fields. Journal of Physical Chemistry Letters, 2017, 8, 3008-3014.	4.6	63
44	Fe thin-film growth on Au(100): A self-surfactant effect and its limitations. Physical Review B, 1999, 59, 15966-15974.	3.2	58
45	Thermodynamic Equilibria in Carbon Nitride Photocatalyst Materials and Conditions for the Existence of Graphitic Carbon Nitride g-C₃N₄. Chemistry of Materials, 2017, 29, 4445-4453.	6.7	58
46	Structural complexity in binary bcc ground states: The case of bcc Mo-Ta. Physical Review B, 2004, 69, .	3.2	56
47	Prediction of ordered structures in the bcc binary systems of Mo, Nb, Ta, and W from first-principles search of approximately 3,000,000 possible configurations. Physical Review B, 2005, 72, .	3.2	53
48	First-principles determination of low-temperature order and ground states of Fe-Ni, Fe-Pd, and Fe-Pt. Physical Review B, 2009, 80, .	3.2	53
49	Large-scale surface reconstruction energetics of Pt(100) and Au(100) by all-electron density functional theory. Physical Review B, 2010, 82, .	3.2	52
50	First-principles data set of 45,892 isolated and cation-coordinated conformers of 20 proteinogenic amino acids. Scientific Data, 2016, 3, 160009.	5.3	51
51	Exploring the conformational preferences of 20-residue peptides in isolation: Ac-Ala₁₉-Lys + H⁺vs. Ac-Lys-Ala₁₉ + H⁺ and the current reach of DFT. Physical Chemistry Chemical Physics, 2015, 17, 7373-7385.	2.8	48
52	Tunable internal quantum well alignment in rationally designed oligomer-based perovskite films deposited by resonant infrared matrix-assisted pulsed laser evaporation. Materials Horizons, 2019, 6, 1707-1716.	12.2	48
53	Structure of thec(2Ã—2)-Br/Pt(110) surface. Physical Review B, 2002, 65, .	3.2	43
54	Validation Challenge of Density-Functional Theory for Peptidesâ€”Example of Ac-Phe-Ala₅-LysH⁺. Journal of Physical Chemistry A, 2014, 118, 7349-7359.	2.5	43

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55	The Structural Origin of Chiroptical Properties in Perovskite Nanocrystals with Chiral Organic Ligands. Advanced Functional Materials, 2022, 32, .	14.9	43
56	Segregation in Strongly Ordering Compounds: A Key Role of Constitutional Defects. Physical Review Letters, 2002, 89, 266102.	7.8	42
57	Isomerism and Structural Fluxionality in the Au₂₆ and Au₂₆^{â€“} Nanoclusters. ACS Nano, 2014, 8, 7413-7422.	14.6	42
58	The role of an energy-dependent inner potential in quantitative low-energy electron diffraction. Surface Science, 2000, 458, 155-161.	1.9	39
59	Segregation phenomena on surfaces of the ordered bimetallic alloy FeAl. Surface Science, 1998, 412-413, 69-81.	1.9	38
60	Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework. Journal of Chemical Physics, 2014, 141, 024105.	3.0	38
61	All-electron ab initio Bethe-Salpeter equation approach to neutral excitations in molecules with numeric atom-centered orbitals. Journal of Chemical Physics, 2020, 152, 044105.	3.0	38
62	How Cations Change Peptide Structure. Chemistry - A European Journal, 2013, 19, 11224-11234.	3.3	36
63	Impact of Vibrational Entropy on the Stability of Unsolvated Peptide Helices with Increasing Length. Journal of Physical Chemistry B, 2013, 117, 5574-5584.	2.6	35
64	Thermodynamic Equilibrium Conditions of Graphene Films on SiC. Physical Review Letters, 2013, 111, 065502.	7.8	34
65	Candidate photoferroic absorber materials for thin-film solar cells from naturally occurring minerals: enargite, stephanite, and bournonite. Sustainable Energy and Fuels, 2017, 1, 1339-1350.	4.9	32
66	Efficient Implicit Solvation Method for Full Potential DFT. Journal of Chemical Theory and Computation, 2017, 13, 5582-5603.	5.3	30
67	GPU acceleration of all-electron electronic structure theory using localized numeric atom-centered basis functions. Computer Physics Communications, 2020, 254, 107314.	7.5	30
68	Length dependence of ionization potentials of transacetylenes: Internally consistent DFT/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m Physical Review B, 2015, 92, .	3.2	28
69	ELSI â€” An open infrastructure for electronic structure solvers. Computer Physics Communications, 2020, 256, 107459.	7.5	27
70	Mechanism of Additive-Assisted Room-Temperature Processing of Metal Halide Perovskite Thin Films. ACS Applied Materials & Interfaces, 2021, 13, 13212-13225.	8.0	27
71	Influence of Annealing and Composition on the Crystal Structure of Mixed-Halide, Ruddlesdenâ€“Popper Perovskites. Chemistry of Materials, 2022, 34, 3109-3122.	6.7	27
72	ORDERED AND DISORDERED RIPPLING IN THE CoAl(110)-(1Ã—1) SURFACE. Surface Review and Letters, 1996, 03, 1409-1415.	1.1	26

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73	Segregation and ordering at Fe1â^'xAlx(100) surfaces â€“ a model case for binary alloys. Surface Science, 2001, 474, 81-97.	1.9	26
74	Resolving Rotational Stacking Disorder and Electronic Level Alignment in a 2D Oligothiophene-Based Lead Iodide Perovskite. Chemistry of Materials, 2019, 31, 8523-8532.	6.7	26
75	Band Gap Tailoring and Structure-Composition Relationship within the Alloyed Semiconductor Cu₂BaGe_{1â€“x}Sn_xSe₄. Chemistry of Materials, 2018, 30, 6566-6574.	6.7	25
76	Structural Tolerance Factor Approach to Defect-Resistant I₂-II-IV-X₄ Semiconductor Design. Chemistry of Materials, 2020, 32, 1636-1649.	6.7	25
77	All-electron periodic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub></mml:mrow> implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. Physical Review Materials, 2021, 5, .	2.4	25
78	Quantitative Subsurface Atomic Structure Fingerprint for 2D Materials and Heterostructures by First-Principles-Calibrated Contact-Resonance Atomic Force Microscopy. ACS Nano, 2016, 10, 6491-6500.	14.6	23
79	Rational ligand choice extends the SABRE substrate scope. Chemical Communications, 2020, 56, 9336-9339.	4.1	23
80	Competitive surface segregation of C, Al and S impurities in Fe(100). Journal of Physics Condensed Matter, 2003, 15, 3517-3529.	1.8	22
81	Trends for isolated amino acids and dipeptides: Conformation, divalent ion binding, and remarkable similarity of binding to calcium and lead. Scientific Reports, 2016, 6, 35772.	3.3	22
82	Water Adsorption at Two Unsolvated Peptides with a Protonated Lysine Residue: From Self-Solvation to Solvation. Journal of Physical Chemistry B, 2012, 116, 14788-14804.	2.6	20
83	All-Electron BSE@GW Method for K-Edge Core Electron Excitation Energies. Journal of Chemical Theory and Computation, 2022, 18, 1569-1583.	5.3	20
84	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
85	GPU-acceleration of the ELPA2 distributed eigensolver for dense symmetric and hermitian eigenproblems. Computer Physics Communications, 2021, 262, 107808.	7.5	19
86	Equilibration processes in surfaces of the binary alloy Fe-Al. Journal of Physics Condensed Matter, 2002, 14, 4145-4164.	1.8	18
87	Thermodynamically accessible titanium clusters Ti_N, N = 2â€“32. Physical Chemistry Chemical Physics, 2018, 20, 13962-13973.	2.8	18
88	Quantification of substitutional disorder and atomic vibrations by LEED â€“ the role of parameter correlations. Surface Science, 2001, 488, 219-232.	1.9	17
89	Structural investigation of nanocrystalline graphene grown on (6âˆš3 Ã— 6âˆš3)R30Â°-reconstructed SiC surfaces by molecular beam epitaxy. New Journal of Physics, 2013, 15, 123034.	2.9	16
90	Relativistic correction scheme for core-level binding energies from GW. Journal of Chemical Physics, 2020, 153, 114110.	3.0	15

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91	Charge transfer states and carrier generation in 1D organolead iodide semiconductors. Journal of Materials Chemistry A, 2021, 9, 14977-14990.	10.3	15
92	Pentacene and tetracene molecules and films on H/Si(111): level alignment from hybrid density functional theory. Electronic Structure, 2020, 2, 035002.	2.8	15
93	On the optical anisotropy in 2D metal-halide perovskites. Nanoscale, 2022, 14, 752-765.	5.6	15
94	Extending holographic LEED to ordered small-unit-cell superstructures. Physical Review B, 1998, 58, 4102-4110.	3.2	14
95	Equilibration of stoichiometrically distorted Fe1-xAlx(100) surfaces. Journal of Physics Condensed Matter, 2001, 13, 1781-1791.	1.8	14
96	Role ofCoantisite segregation in theCoAl(111)surface. Physical Review B, 2005, 71, .	3.2	14
97	Native like helices in a specially designed Î² peptide in the gas phase. Physical Chemistry Chemical Physics, 2015, 17, 5376-5385.	2.8	14
98	All-electron real-time and imaginary-time time-dependent density functional theory within a numeric atom-centered basis function framework. Journal of Chemical Physics, 2021, 155, 154801.	3.0	14
99	Why graphene growth is very different on the C face than on the Si face of SiC: Insights from surface equilibria and the<mml:math		

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109	MatD^3^: A Database and Online Presentation Package for Research Data Supporting Materials Discovery, Design, and Dissemination. Journal of Open Source Software, 2020, 5, 1945.	4.6	2
110	Publisher's Note: Prediction of ordered structures in the bcc binary systems of Mo, Nb, Ta, and W from first-principles search of approximately 3,000,000 possible configurations [Phys. Rev. B72, 020104(R) (2005)]. Physical Review B, 2005, 72, .	3.2	1
111	Accurate frozen core approximation for all-electron density-functional theory. Journal of Chemical Physics, 2021, 154, 224107.	3.0	1
112	GIMS: Graphical Interface for Materials Simulations. Journal of Open Source Software, 2021, 6, 2767.	4.6	1
113	Boron nitride on SiC(0001). Physical Review Materials, 2022, 6, .	2.4	1
114	How mono-valent cations bend peptide turns and a first-principles database of amino acids and dipeptides. , 2014, , .		0