Volker Blum

List of Publications by Year
in descending order

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Version: 2024-02-01

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	On the optical anisotropy in 2D metal-halide perovskites. Nanoscale, 2022, 14, 752-765.	5.6	15
2	Cubic Crystal Structure Formation and Optical Properties within the Agâ€“B^{II}â€“M^{IV}â€“X (B^{II} = Sr, Pb; M^{IV} = Si, Ge, Sn; X = S, Se) Family of Semiconductors. Inorganic Chemistry, 2022, 61, 2929-2944.	4.0	3
3	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
4	The Structural Origin of Chiroptical Properties in Perovskite Nanocrystals with Chiral Organic Ligands. Advanced Functional Materials, 2022, 32, .	14.9	43
5	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
6	Nuclearâ€“electronic orbital approach to quantization of protons in periodic electronic structure calculations. Journal of Chemical Physics, 2022, 156, .	3.0	3
7	Boron nitride on SiC(0001). Physical Review Materials, 2022, 6, .	2.4	1
8	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:m implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. Physical Review Materials, 2021, 5, .	2.4	25
9	Charge transfer states and carrier generation in 1D organolead iodide semiconductors. Journal of Materials Chemistry A, 2021, 9, 14977-14990.	10.3	15
10	Mechanism of Additive-Assisted Room-Temperature Processing of Metal Halide Perovskite Thin Films. ACS Applied Materials & Interfaces, 2021, 13, 13212-13225.	8.0	27
11	GPU-acceleration of the ELPA2 distributed eigensolver for dense symmetric and hermitian eigenproblems. Computer Physics Communications, 2021, 262, 107808.	7.5	19
12	Accurate frozen core approximation for all-electron density-functional theory. Journal of Chemical Physics, 2021, 154, 224107.	3.0	1
13	Quasi-four-component method with numeric atom-centered orbitals for relativistic density functional simulations of molecules and solids. Physical Review B, 2021, 103, .	3.2	7
14	Structural, Optical, and Electronic Properties of Two Quaternary Chalcogenide Semiconductors: Ag₂SrSiS₄ and Ag₂SrGeS₄. Inorganic Chemistry, 2021, 60, 12206-12217.	4.0	8
15	Structural descriptor for enhanced spin-splitting in 2D hybrid perovskites. Nature Communications, 2021, 12, 4982.	12.8	78
16	Density Functional Theory Study of Reaction Equilibria in Signal Amplification by Reversible Exchange. ChemPhysChem, 2021, 22, 1947-1957.	2.1	8
17	GIMS: Graphical Interface for Materials Simulations. Journal of Open Source Software, 2021, 6, 2767.	4.6	1
18	Density Functional Theory Study of Reaction Equilibria in Signal Amplification by Reversible Exchange. ChemPhysChem, 2021, 22, 1937-1938.	2.1	2

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19	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
20	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
21	Trapping lead in perovskite solar modules with abundant and low-cost cation-exchange resins. Nature Energy, 2020, 5, 1003-1011.	39.5	126
22	Relativistic correction scheme for core-level binding energies from GW. Journal of Chemical Physics, 2020, 153, 114110.	3.0	15
23	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
24	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
25	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589
26	ELSI â€" An open infrastructure for electronic structure solvers. Computer Physics Communications, 2020, 256, 107459.	7.5	27
27	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
28	Structural Tolerance Factor Approach to Defect-Resistant I₂-II-IV-X₄ Semiconductor Design. Chemistry of Materials, 2020, 32, 1636-1649.	6.7	25
29	Frenkelâ€"Holstein Hamiltonian applied to absorption spectra of quaterthiophene-based 2D hybrid organicâ€"inorganic perovskites. Journal of Chemical Physics, 2020, 152, 144702.	3.0	8
30	GPU acceleration of all-electron electronic structure theory using localized numeric atom-centered basis functions. Computer Physics Communications, 2020, 254, 107314.	7.5	30
31	Rational ligand choice extends the SABRE substrate scope. Chemical Communications, 2020, 56, 9336-9339.	4.1	23
32	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
33	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
34	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
35	Molecular engineering of organicâ€"inorganic hybrid perovskites quantum wells. Nature Chemistry, 2019, 11, 1151-1157.	13.6	302
36	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

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37	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
38	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
39	Formation of graphene atop a Si adlayer on the C-face of SiC. Physical Review Materials, 2019, 3, .	2.4	3
40	Thermodynamically accessible titanium clusters Ti_N, N = 2â€“32. Physical Chemistry Chemical Physics, 2018, 20, 13962-13973.	2.8	18
41	ELSI: A unified software interface for Kohnâ€“Sham electronic structure solvers. Computer Physics Communications, 2018, 222, 267-285.	7.5	78
42	Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites. Physical Review Letters, 2018, 121, 146401.	7.8	103
43	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
44	Ureaâ€Modified Carbon Nitrides: Enhancing Photocatalytic Hydrogen Evolution by Rational Defect Engineering. Advanced Energy Materials, 2017, 7, 1602251.	19.5	238
45	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
46	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
47	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
48	The Elephant in the Room of Density Functional Theory Calculations. Journal of Physical Chemistry Letters, 2017, 8, 1449-1457.	4.6	88
49	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
50	Efficient Implicit Solvation Method for Full Potential DFT. Journal of Chemical Theory and Computation, 2017, 13, 5582-5603.	5.3	30
51	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
52	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
53	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
54	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

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55	Rational design of carbon nitride photocatalysts by identification of cyanamide defects as catalytically relevant sites. Nature Communications, 2016, 7, 12165.	12.8	586
56	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
57	BaCu₂Sn(S,Se)₄: Earth-Abundant Chalcogenides for Thin-Film Photovoltaics. Chemistry of Materials, 2016, 28, 4771-4780.	6.7	131
58	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
59	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
60	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
61	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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73	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
74	Isomerism and Structural Fluxionality in the Au₂₆ and Au₂₆^{â€“} Nanoclusters. ACS Nano, 2014, 8, 7413-7422.	14.6	42
75	Thermodynamic Equilibrium Conditions of Graphene Films on SiC. Physical Review Letters, 2013, 111, 065502.	7.8	34
76	How Cations Change Peptide Structure. Chemistry - A European Journal, 2013, 19, 11224-11234.	3.3	36
77	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
78	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
79	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
80	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. New Journal of Physics, 2013, 15, 123033.	2.9	81
81	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
82	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
83	Parallel solution of partial symmetric eigenvalue problems from electronic structure calculations. Parallel Computing, 2011, 37, 783-794.	2.1	147
84	Unraveling the Stability of Polypeptide Helices: Critical Role of van der Waals Interactions. Physical Review Letters, 2011, 106, 118102.	7.8	97
85	Secondary Structure of Ac-Ala_n-LysH⁺ Polyalanine Peptides (n =) Tj ETQq1 1 0.784314 rgBT /Ov	4.6	76
86	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
87	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
88	Efficient integration for all-electron electronic structure calculation using numeric basis functions. Journal of Computational Physics, 2009, 228, 8367-8379.	3.8	454
89	Ab initio molecular simulations with numeric atom-centered orbitals. Computer Physics Communications, 2009, 180, 2175-2196.	7.5	2,170
90	Accuracy of first-principles lateral interactions: Oxygen at Pd(100). Physical Review B, 2007, 75, .	3.2	83

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91	The surface oxide: A LEED, DFT and STM study. Surface Science, 2007, 601, 1574-1581.	1.9	96
92	Prediction of unusual stable ordered structures of Au-Pd alloys via a first-principles cluster expansion. Physical Review B, 2006, 74, .	3.2	71
93	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
94	Evolutionary approach for determining first-principles hamiltonians. Nature Materials, 2005, 4, 391-394.	27.5	285
95	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
96	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
97	Role ofCoantisite segregation in theCoAl(111)surface. Physical Review B, 2005, 71, .	3.2	14
98	Structural complexity in binary bcc ground states: The case of bcc Mo-Ta. Physical Review B, 2004, 69, .	3.2	56
99	Mixed-basis cluster expansion for thermodynamics of bcc alloys. Physical Review B, 2004, 70, .	3.2	95
100	The Pd()â€“R27Â°-O surface oxide revisited. Surface Science, 2003, 541, 101-112.	1.9	201
101	Competitive surface segregation of C, Al and S impurities in Fe(100). Journal of Physics Condensed Matter, 2003, 15, 3517-3529.	1.8	22
102	Segregation in Strongly Ordering Compounds: A Key Role of Constitutional Defects. Physical Review Letters, 2002, 89, 266102.	7.8	42
103	Structure of thec(2Ã—2)-Br/Pt(110) surface. Physical Review B, 2002, 65, .	3.2	43
104	Equilibration processes in surfaces of the binary alloy Fe-Al. Journal of Physics Condensed Matter, 2002, 14, 4145-4164.	1.8	18
105	Segregation and ordering at Fe1â^'xAlx(100) surfaces â€“ a model case for binary alloys. Surface Science, 2001, 474, 81-97.	1.9	26
106	Quantification of substitutional disorder and atomic vibrations by LEED â€“ the role of parameter correlations. Surface Science, 2001, 488, 219-232.	1.9	17
107	Fast LEED intensity calculations for surface crystallography using Tensor LEED. Computer Physics Communications, 2001, 134, 392-425.	7.5	119
108	Equilibration of stoichiometrically distorted Fe1-xAlx(100) surfaces. Journal of Physics Condensed Matter, 2001, 13, 1781-1791.	1.8	14

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109	The role of an energy-dependent inner potential in quantitative low-energy electron diffraction. Surface Science, 2000, 458, 155-161.	1.9	39
110	Fe thin-film growth on Au(100): A self-surfactant effect and its limitations. Physical Review B, 1999, 59, 15966-15974.	3.2	58
111	Segregation phenomena on surfaces of the ordered bimetallic alloy FeAl. Surface Science, 1998, 412-413, 69-81.	1.9	38
112	Extending holographic LEED to ordered small-unit-cell superstructures. Physical Review B, 1998, 58, 4102-4110.	3.2	14
113	ORDERED AND DISORDERED RIPPLING IN THE CoAl(110)-(1Ã—1) SURFACE. Surface Review and Letters, 1996, 03, 1409-1415.	1.1	26
114	The Auger (autoionization) spectra excited by argon and neon ion bombardment of a magnesium surface. Journal of Physics Condensed Matter, 1994, 6, 9677-9688.	1.8	6