Volker Blum

List of Publications by Citations

109 papers	8,648 citations	46 h-index	92 g-index
120 ext. papers	10,331 ext. citations	7 avg, IF	5.98 L-index

#	Paper	IF	Citations
109	Ab initio molecular simulations with numeric atom-centered orbitals. *Computer Physics Communications*, **2009**, 180, 2175-2196	4.2	1637
108	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
107	Rational design of carbon nitride photocatalysts by identification of cyanamide defects as catalytically relevant sites. *Nature Communications*, **2016**, 7, 12165	17.4	417
106	Resolution-of-identity approach to Hartree–Fock, hybrid density functionals, RPA, MP2 andGWwith numeric atom-centered orbital basis functions. *New Journal of Physics*, **2012**, 14, 053020	2.9	411
105	Efficient O(N) integration for all-electron electronic structure calculation using numeric basis functions. *Journal of Computational Physics*, **2009**, 228, 8367-8379	4.1	342
104	Low-molecular-weight carbon nitrides for solar hydrogen evolution. *Journal of the American Chemical Society*, **2015**, 137, 1064-72	16.4	267
103	Evolutionary approach for determining first-principles hamiltonians. *Nature Materials*, **2005**, 4, 391-4	27	249
102	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *Journal of Chemical Physics*, **2020**, 152, 124101	3.9	210
101	The Pd()R27°-O surface oxide revisited. *Surface Science*, **2003**, 541, 101-112	1.8	185
100	Urea-Modified Carbon Nitrides: Enhancing Photocatalytic Hydrogen Evolution by Rational Defect Engineering. *Advanced Energy Materials*, **2017**, 7, 1602251	21.8	174
99	Direct and cost-efficient hyperpolarization of long-lived nuclear spin states on universal (15)N2-diazirine molecular tags. *Science Advances*, **2016**, 2, e1501438	14.3	167
98	Molecular engineering of organic-inorganic hybrid perovskites quantum wells. *Nature Chemistry*, **2019**, 11, 1151-1157	17.6	160
97	Parallel solution of partial symmetric eigenvalue problems from electronic structure calculations. *Parallel Computing*, **2011**, 37, 783-794	1	124
96	The ELPA library: scalable parallel eigenvalue solutions for electronic structure theory and computational science. *Journal of Physics Condensed Matter*, **2014**, 26, 213201	1.8	116
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,	3.3	115
94	Fast LEED intensity calculations for surface crystallography using Tensor LEED. *Computer Physics Communications*, **2001**, 134, 392-425	4.2	109
93	BaCu2Sn(S,Se)4: Earth-Abundant Chalcogenides for Thin-Film Photovoltaics. *Chemistry of Materials*, **2016**, 28, 4771-4780	9.6	101

92	Isomer-selective detection of hydrogen-bond vibrations in the protonated water hexamer. *Journal of the American Chemical Society*, **2013**, 135, 8266-73	16.4	101
91	Direct-Bandgap 2D Silver-Bismuth Iodide Double Perovskite: The Structure-Directing Influence of an Oligothiophene Spacer Cation. *Journal of the American Chemical Society*, **2019**, 141, 7955-7964	16.4	100
90	Unraveling the stability of polypeptide helices: critical role of van der Waals interactions. *Physical Review Letters*, **2011**, 106, 118102	7.4	90
89	The surface oxide: A LEED, DFT and STM study. *Surface Science*, **2007**, 601, 1574-1581	1.8	90
88	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. *Computer Physics Communications*, **2015**, 192, 60-69	4.2	89
87	Earth-Abundant Chalcogenide Photovoltaic Devices with over 5% Efficiency Based on a Cu BaSn(S,Se) Absorber. *Advanced Materials*, **2017**, 29, 1606945	24	85
86	Mixed-basis cluster expansion for thermodynamics of bcc alloys. *Physical Review B*, **2004**, 70,	3.3	82
85	Highly Distorted Chiral Two-Dimensional Tin Iodide Perovskites for Spin Polarized Charge Transport. *Journal of the American Chemical Society*, **2020**, 142, 13030-13040	16.4	79
84	Accuracy of first-principles lateral interactions: Oxygen at Pd(100). *Physical Review B*, **2007**, 75,	3.3	77
83	Secondary Structure of Ac-Alan-LysH+ Polyalanine Peptides (n = 5,10,15) in Vacuo: Helical or Not?. *Journal of Physical Chemistry Letters*, **2010**, 1, 3465-3470	6.4	72
82	Siesta: Recent developments and applications. *Journal of Chemical Physics*, **2020**, 152, 204108	3.9	69
81	I2□□V□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	9.6	67
80	Prediction of unusual stable ordered structures of Au-Pd alloys via a first-principles cluster expansion. *Physical Review B*, **2006**, 74,	3.3	66
79	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	65
78	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. *New Journal of Physics*, **2013**, 15, 123033	2.9	65
77	Trapping lead in perovskite solar modules with abundant and low-cost cation-exchange resins. *Nature Energy*, **2020**, 5, 1003-1011	62.3	65
76	Organic-to-inorganic structural chirality transfer in a 2D hybrid perovskite and impact on Rashba-Dresselhaus spin-orbit coupling. *Nature Communications*, **2020**, 11, 4699	17.4	65
75	Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites. *Physical Review Letters*, **2018**, 121, 146401	7.4	65

74	First-Principles Molecular Structure Search with a Genetic Algorithm. *Journal of Chemical Information and Modeling*, **2015**, 55, 2338-48	6.1	61
73	The Elephant in the Room of Density Functional Theory Calculations. *Journal of Physical Chemistry Letters*, **2017**, 8, 1449-1457	6.4	60
72	Approaching truly freestanding graphene: the structure of hydrogen-intercalated graphene on 6H-SiC(0001). *Physical Review Letters*, **2015**, 114, 106804	7.4	59
71	All-electron formalism for total energy strain derivatives and stress tensor components for numeric atom-centered orbitals. *Computer Physics Communications*, **2015**, 190, 33-50	4.2	58
70	Fe thin-film growth on Au(100): A self-surfactant effect and its limitations. *Physical Review B*, **1999**, 59, 15966-15974	3.3	58
69	Long-Lived C Nuclear Spin States Hyperpolarized by Parahydrogen in Reversible Exchange at Microtesla Fields. *Journal of Physical Chemistry Letters*, **2017**, 8, 3008-3014	6.4	55
68	Structural complexity in binary bcc ground states: The case of bcc Mo-Ta. *Physical Review B*, **2004**, 69,	3.3	53
67	One-hundred-three compound band-structure benchmark of post-self-consistent spin-orbit coupling treatments in density functional theory. *Physical Review Materials*, **2017**, 1,	3.2	52
66	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,	3.3	47
65	Large-scale surface reconstruction energetics of Pt(100) and Au(100) by all-electron density functional theory. *Physical Review B*, **2010**, 82,	3.3	46
64	First-principles determination of low-temperature order and ground states of Fe-Ni, Fe-Pd, and Fe-Pt. *Physical Review B*, **2009**, 80,	3.3	46
63	ELSI: A unified software interface for Kohn□Sham electronic structure solvers. *Computer Physics Communications*, **2018**, 222, 267-285	4.2	43
62	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, 7373-85	3.6	42
61	Segregation in strongly ordering compounds: a key role of constitutional defects. *Physical Review Letters*, **2002**, 89, 266102	7.4	41
60	Isomerism and structural fluxionality in the Au26 and Au26(-) nanoclusters. *ACS Nano*, **2014**, 8, 7413-22	16.7	40
59	Structure of the c(2□)-Br/Pt(110) surface. *Physical Review B*, **2002**, 65,	3.3	40
58	First-principles data set of 45,892 isolated and cation-coordinated conformers of 20 proteinogenic amino acids. *Scientific Data*, **2016**, 3, 160009	8.2	39
57	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	9.6	38

56	Validation challenge of density-functional theory for peptides-example of Ac-Phe-Ala5-LysH(+). *Journal of Physical Chemistry A*, **2014**, 118, 7349-59	2.8	38
55	Segregation phenomena on surfaces of the ordered bimetallic alloy FeAl. *Surface Science*, **1998**, 412-413, 69-81	1.8	38
54	The role of an energy-dependent inner potential in quantitative low-energy electron diffraction. *Surface Science*, **2000**, 458, 155-161	1.8	35
53	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	14.4	34
52	Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework. *Journal of Chemical Physics*, **2014**, 141, 024105	3.9	33
51	Thermodynamic equilibrium conditions of graphene films on SiC. *Physical Review Letters*, **2013**, 111, 065502	7.4	32
50	How cations change peptide structure. *Chemistry - A European Journal*, **2013**, 19, 11224-34	4.8	32
49	Impact of vibrational entropy on the stability of unsolvated peptide helices with increasing length. *Journal of Physical Chemistry B*, **2013**, 117, 5574-84	3.4	28
48	ORDERED AND DISORDERED RIPPLING IN THE CoAl(110)-(1□) SURFACE. *Surface Review and Letters*, **1996**, 03, 1409-1415	1.1	26
47	Length dependence of ionization potentials of transacetylenes: Internally consistent DFT/GW approach. *Physical Review B*, **2015**, 92,	3.3	25
46	Segregation and ordering at Fe1□Alx(100) surfaces □ a model case for binary alloys. *Surface Science*, **2001**, 474, 81-97	1.8	25
45	Efficient Implicit Solvation Method for Full Potential DFT. *Journal of Chemical Theory and Computation*, **2017**, 13, 5582-5603	6.4	24
44	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	5.8	23
43	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	3.9	22
42	Competitive surface segregation of C, Al and S impurities in Fe(100). *Journal of Physics Condensed Matter*, **2003**, 15, 3517-3529	1.8	21
41	Quantitative Subsurface Atomic Structure Fingerprint for 2D Materials and Heterostructures by First-Principles-Calibrated Contact-Resonance Atomic Force Microscopy. *ACS Nano*, **2016**, 10, 6491-500	16.7	19
40	Equilibration processes in surfaces of the binary alloy Fe-Al. *Journal of Physics Condensed Matter*, **2002**, 14, 4145-4164	1.8	18
39	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	4.9	18

38	Quantification of substitutional disorder and atomic vibrations by LEED □the role of parameter correlations. *Surface Science*, **2001**, 488, 219-232	1.8	17
37	Band Gap Tailoring and Structure-Composition Relationship within the Alloyed Semiconductor Cu2BaGe1□SnxSe4. *Chemistry of Materials*, **2018**, 30, 6566-6574	9.6	17
36	Water adsorption at two unsolvated peptides with a protonated lysine residue: from self-solvation to solvation. *Journal of Physical Chemistry B*, **2012**, 116, 14788-804	3.4	16
35	Rational ligand choice extends the SABRE substrate scope. *Chemical Communications*, **2020**, 56, 9336-9339	3.8	15
34	Resolving Rotational Stacking Disorder and Electronic Level Alignment in a 2D Oligothiophene-Based Lead Iodide Perovskite. *Chemistry of Materials*, **2019**, 31, 8523-8532	9.6	14
33	ELSI □An open infrastructure for electronic structure solvers. *Computer Physics Communications*, **2020**, 256, 107459	4.2	14
32	Structural Tolerance Factor Approach to Defect-Resistant I2-II-IV-X4 Semiconductor Design. *Chemistry of Materials*, **2020**, 32, 1636-1649	9.6	14
31	Role of Co antisite segregation in the CoAl(111) surface. *Physical Review B*, **2005**, 71,	3.3	14
30	Equilibration of stoichiometrically distorted Fe1-xAlx(100) surfaces. *Journal of Physics Condensed Matter*, **2001**, 13, 1781-1791	1.8	14
29	Extending holographic LEED to ordered small-unit-cell superstructures. *Physical Review B*, **1998**, 58, 4102-4110	3.3	14
28	GPU acceleration of all-electron electronic structure theory using localized numeric atom-centered basis functions. *Computer Physics Communications*, **2020**, 254, 107314	4.2	14
27	Native like helices in a specially designed □peptide in the gas phase. *Physical Chemistry Chemical Physics*, **2015**, 17, 5376-85	3.6	13
26	Structural investigation of nanocrystalline graphene grown on (6□ 6□)R30°-reconstructed SiC surfaces by molecular beam epitaxy. *New Journal of Physics*, **2013**, 15, 123034	2.9	13
25	Mechanism of Additive-Assisted Room-Temperature Processing of Metal Halide Perovskite Thin Films. *ACS Applied Materials & Interfaces*, **2021**, 13, 13212-13225	9.5	13
24	Structural descriptor for enhanced spin-splitting in 2D hybrid perovskites. *Nature Communications*, **2021**, 12, 4982	17.4	13
23	Why graphene growth is very different on the C face than on the Si face of SiC: Insights from surface equilibria and the (3□)□C□SiC(1□1□1□) reconstruction. *Physical Review B*, **2015**, 91,	3.3	11
22	All-electron periodic G0W0 implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. *Physical Review Materials*, **2021**, 5,	3.2	11
21	Thermodynamically accessible titanium clusters Ti, N = 2-32. *Physical Chemistry Chemical Physics*, **2018**, 20, 13962-13973	3.6	10

20	Relativistic correction scheme for core-level binding energies from GW. *Journal of Chemical Physics*, **2020**, 153, 114110	3.9	10
19	The Structural Origin of Chiroptical Properties in Perovskite Nanocrystals with Chiral Organic Ligands. *Advanced Functional Materials*,2200454	15.6	8
18	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
17	Pentacene and tetracene molecules and films on H/Si(111): level alignment from hybrid density functional theory. *Electronic Structure*, **2020**, 2, 035002	2.6	6
16	The CECAM electronic structure library and the modular software development paradigm. *Journal of Chemical Physics*, **2020**, 153, 024117	3.9	5
15	GPU-acceleration of the ELPA2 distributed eigensolver for dense symmetric and hermitian eigenproblems. *Computer Physics Communications*, **2021**, 262, 107808	4.2	5
14	On the optical anisotropy in 2D metal-halide perovskites.. *Nanoscale*, **2021**,	7.7	3
13	Formation of graphene atop a Si adlayer on the C-face of SiC. *Physical Review Materials*, **2019**, 3,	3.2	3
12	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	3.9	3
11	Charge transfer states and carrier generation in 1D organolead iodide semiconductors. *Journal of Materials Chemistry A*, **2021**, 9, 14977-14990	13	3
10	Frenkel-Holstein Hamiltonian applied to absorption spectra of quaterthiophene-based 2D hybrid organic-inorganic perovskites. *Journal of Chemical Physics*, **2020**, 152, 144702	3.9	2
9	Density Functional Theory Study of Reaction Equilibria in Signal Amplification by Reversible Exchange. *ChemPhysChem*, **2021**, 22, 1937-1938	3.2	2
8	Quasi-four-component method with numeric atom-centered orbitals for relativistic density functional simulations of molecules and solids. *Physical Review B*, **2021**, 103,	3.3	2
7	Structural, Optical, and Electronic Properties of Two Quaternary Chalcogenide Semiconductors: AgSrSiS and AgSrGeS. *Inorganic Chemistry*, **2021**, 60, 12206-12217	5.1	2
6	Density Functional Theory Study of Reaction Equilibria in Signal Amplification by Reversible Exchange. *ChemPhysChem*, **2021**, 22, 1947-1957	3.2	2
5	All-Electron BSE@ Method for -Edge Core Electron Excitation Energies.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	1
4	Cubic Crystal Structure Formation and Optical Properties within the Ag-B-M-X (B = Sr, Pb; M = Si, Ge, Sn; X = S, Se) Family of Semiconductors.. *Inorganic Chemistry*, **2022**, 61, 2929-2944	5.1	0
3	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	5.2	0

2	Accurate frozen core approximation for all-electron density-functional theory. *Journal of Chemical Physics*, **2021**, 154, 224107	3.9
1	GIMS: Graphical Interface for Materials Simulations. *Journal of Open Source Software*, **2021**, 6, 2767	5.2