T BjÃ¶rkman

List of Publications by Year
in descending order

40 papers	4,590 citations	279487 23 h-index	288905 40 g-index
40 all docs	40 docs citations	40 times ranked	8376 citing authors

#	Article	IF	Citations
1	Realistic first-principles calculations of the magnetocaloric effect: applications to hcp Gd. Materials Research Letters, 2022, 10, 156-162.	4.1	4
2	High-throughput and data-mining approach to predict new rare-earth free permanent magnets. Physical Review B, 2020, 101, .	1.1	34
3	Electronic properties of several two dimensional halides from ab initio calculations. Beilstein Journal of Nanotechnology, 2019, 10, 823-832.	1.5	24
4	Advances in Density-Functional Calculations for Materials Modeling. Annual Review of Materials Research, 2019, 49, 1-30.	4.3	87
5	Effects of electron beam-generated lattice defects on the periodic lattice distortion structure in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â^'	1.1	7
6	Observation of charge density waves in free-standing 1T-TaSe2 monolayers by transmission electron microscopy. Applied Physics Letters, 2018, 113, .	1.5	24
7	Substitutional carbon doping of free-standing and Ru-supported BN sheets: a first-principles study. Journal of Physics Condensed Matter, 2017, 29, 415301.	0.7	5
8	Effect of Magnetic Ordering on the Stability of Niâ€“Mnâ€“Ga(â€“Coâ€“Cu) Alloys Along the Tetragonal Deformation Path. IEEE Transactions on Magnetics, 2017, 53, 1-6.	1.2	3
9	Combining electronic structure and many-body theory with large databases: A method for predicting the nature of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi></mml:mrow></mml:m states in Ce compounds. Physical Review Materials, 2017, 1, .	0.9	16
10	2D Structures Beyond Graphene. Semiconductors and Semimetals, 2016, 95, 1-33.	0.4	8
11	First-principles investigation of two-dimensional trichalcogenide and sesquichalcogenide monolayers. Physical Review B, 2016, 93, .	1.1	44
12	Vibrational Properties of a Two-Dimensional Silica Kagome Lattice. ACS Nano, 2016, 10, 10929-10935.	7.3	18
13	Van der Waals interactions and the limits of isolated atom models at interfaces. Nature Communications, 2016, 7, 11559.	5.8	111
14	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
15	Ab Initio Study of Properties of Co- and Cu- Doped Ni-Mn-Ga Alloys. Materials Today: Proceedings, 2015, 2, S601-S604.	0.9	8
16	Solubility of Boron, Carbon, and Nitrogen in Transition Metals: Getting Insight into Trends from First-Principles Calculations. Journal of Physical Chemistry Letters, 2015, 6, 3263-3268.	2.1	50
17	Three-fold rotational defects in two-dimensional transition metal dichalcogenides. Nature Communications, 2015, 6, 6736.	5.8	179
18	Single-Layer ReS₂: Two-Dimensional Semiconductor with Tunable In-Plane Anisotropy. ACS Nano, 2015, 9, 11249-11257.	7.3	353

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19	Testing several recent van der Waals density functionals for layered structures. Journal of Chemical Physics, 2014, 141, 074708.	1.2	145
20	First-principles study of Co- and Cu-doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Ni</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:n the tetragonal deformation path. Physical Review B, 2014, 89, .	1.1	23
21	Triazineâ€Based Graphitic Carbon Nitride: a Twoâ€Dimensional Semiconductor. Angewandte Chemie - International Edition, 2014, 53, 7450-7455.	7.2	523
22	Toward Stronger Alâ€“BN Nanotube Composite Materials: Insights into Bonding at the Al/BN Interface from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 26894-26901.	1.5	24
23	Solid-State Growth of One- and Two-Dimensional Silica Structures on Metal Surfaces. Journal of Physical Chemistry C, 2014, 118, 21001-21005.	1.5	7
24	Launching the Theoretical Crystallography Open Database. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1736-C1736.	0.0	6
25	Two-Dimensional Materials from Data Filtering andAb InitioCalculations. Physical Review X, 2013, 3, .	2.8	180
26	Electronic structure and magnetic properties of Mn, Co, and Ni substitution of Fe in Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>N. Physical Review B, 2013, 88, .	1.1	29
27	Defects in bilayer silica and graphene: common trends in diverse hexagonal two-dimensional systems. Scientific Reports, 2013, 3, 3482.	1.6	80
28	In Situ Growth of Cellular Two-Dimensional Silicon Oxide on Metal Substrates. ACS Nano, 2013, 7, 5175-5180.	7.3	31
29	Charge self-consistent dynamical mean-field theory based on the full-potential linear muffin-tin orbital method: Methodology and applications. Computational Materials Science, 2012, 55, 295-302.	1.4	98
30	van der Waals density functional for solids. Physical Review B, 2012, 86, .	1.1	74
31	Are we van der Waals ready?. Journal of Physics Condensed Matter, 2012, 24, 424218.	0.7	129
32	van der Waals Bonding in Layered Compounds from Advanced Density-Functional First-Principles Calculations. Physical Review Letters, 2012, 108, 235502.	2.9	851
33	High-temperature phonon stabilization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î³</mml:mi></mml:math>-uranium from relativistic first-principles theory. Physical Review B, 2012, 85, .	1.1	59
34	CIF2Cell: Generating geometries for electronic structure programs. Computer Physics Communications, 2011, 182, 1183-1186.	3.0	128
35	Adaptive smearing for Brillouin zone integration. International Journal of Quantum Chemistry, 2011, 111, 1025-1030.	1.0	13
36	Order-disorder induced magnetic structures of FeMnP0.75Si0.25. Physical Review B, 2011, 83, .	1.1	27

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37	Theoretical studies of the incommensurate magnetic structure of a heavy fermion system:CeRhIn5. Physical Review B, 2010, 81, .	1.1	4
38	Dynamical stabilization of the body centered cubic phase in lanthanum and thorium by phononâ€“phonon interaction. Journal of Physics Condensed Matter, 2009, 21, 175402.	0.7	12
39	Coupling between the4fcore binding energy and the5fvalence band occupation of elemental Pu and Pu-based compounds. Physical Review B, 2008, 78, .	1.1	7
40	Crystal and magnetic structure investigation ofTbNi5â^'xCux(x=0,0.5,1.0,1.5,2.0): Experiment and theory. Physical Review B, 2006, 74, .	1.1	22