

List of Publications by Year in descending order

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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	Reproducibility in density functional theory calculations of solids. <i>Science</i> , 2016, 351, aad3000.	6.0	1,113
2	van der Waals Bonding in Layered Compounds from Advanced Density-Functional First-Principles Calculations. <i>Physical Review Letters</i> , 2012, 108, 235502.	2.9	851
3	Triazine-Based Graphitic Carbon Nitride: a Two-Dimensional Semiconductor. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 7450-7455.	7.2	523
4	Single-Layer ReS ₂ : Two-Dimensional Semiconductor with Tunable In-Plane Anisotropy. <i>ACS Nano</i> , 2015, 9, 11249-11257.	7.3	353
5	Two-Dimensional Materials from Data Filtering and <i>Ab Initio</i> Calculations. <i>Physical Review X</i> , 2013, 3, .	2.8	180
6	Three-fold rotational defects in two-dimensional transition metal dichalcogenides. <i>Nature Communications</i> , 2015, 6, 6736.	5.8	179
7	Testing several recent van der Waals density functionals for layered structures. <i>Journal of Chemical Physics</i> , 2014, 141, 074708.	1.2	145
8	Are we van der Waals ready?. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 424218.	0.7	129
9	CF2Cell: Generating geometries for electronic structure programs. <i>Computer Physics Communications</i> , 2011, 182, 1183-1186.	3.0	128
10	Van der Waals interactions and the limits of isolated atom models at interfaces. <i>Nature Communications</i> , 2016, 7, 11559.	5.8	111
11	Charge self-consistent dynamical mean-field theory based on the full-potential linear muffin-tin orbital method: Methodology and applications. <i>Computational Materials Science</i> , 2012, 55, 295-302.	1.4	98
12	Advances in Density-Functional Calculations for Materials Modeling. <i>Annual Review of Materials Research</i> , 2019, 49, 1-30.	4.3	87
13	Defects in bilayer silica and graphene: common trends in diverse hexagonal two-dimensional systems. <i>Scientific Reports</i> , 2013, 3, 3482.	1.6	80
14	van der Waals density functional for solids. <i>Physical Review B</i> , 2012, 86, .	1.1	74
15	High-temperature phonon stabilization of γ -uranium from relativistic first-principles theory. <i>Physical Review B</i> , 2012, 85, .	1.1	59
16	First-principles study of Co- and Cu-doped NiMn ₂ Sb and the tetragonal deformation path. <i>Physical Review B</i> , 2014, 89, .	1.1	55
17	Solubility of Boron, Carbon, and Nitrogen in Transition Metals: Getting Insight into Trends from First-Principles Calculations. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3263-3268.	2.1	50
18	First-principles investigation of two-dimensional trichalcogenide and sesquichalcogenide monolayers. <i>Physical Review B</i> , 2016, 93, .	1.1	44

#	ARTICLE	IF	CITATIONS
19	High-throughput and data-mining approach to predict new rare-earth free permanent magnets. Physical Review B, 2020, 101, .	1.1	34
20	<i>In Situ</i> Growth of Cellular Two-Dimensional Silicon Oxide on Metal Substrates. ACS Nano, 2013, 7, 5175-5180.	7.3	31
21	Electronic structure and magnetic properties of Mn, Co, and Ni substitution of Fe in Fe ₄ N. Physical Review B, 2013, 88, .	1.1	29
22	Order-disorder induced magnetic structures of FeMnP _{0.75} Si _{0.25} . Physical Review B, 2011, 83, .	1.1	27
23	Toward Stronger Al-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
24	Observation of charge density waves in free-standing 1T-TaSe ₂ monolayers by transmission electron microscopy. Applied Physics Letters, 2018, 113, .	1.5	24
25	Electronic properties of several two dimensional halides from ab initio calculations. Beilstein Journal of Nanotechnology, 2019, 10, 823-832.	1.5	24
26	Crystal and magnetic structure investigation of TbNi _{5-x} Cu _x (x=0,0.5,1.0,1.5,2.0): Experiment and theory. Physical Review B, 2006, 74, .	1.1	22
27	Vibrational Properties of a Two-Dimensional Silica Kagome Lattice. ACS Nano, 2016, 10, 10929-10935.	7.3	18
28	Combining electronic structure and many-body theory with large databases: A method for predicting the nature of f states in Ce compounds. Physical Review Materials, 2017, 1, .	0.9	16
29	Adaptive smearing for Brillouin zone integration. International Journal of Quantum Chemistry, 2011, 111, 1025-1030.	1.0	13
30	Dynamical stabilization of the body centered cubic phase in lanthanum and thorium by phonon-phonon interaction. Journal of Physics Condensed Matter, 2009, 21, 175402.	0.7	12
31	Ab Initio Study of Properties of Co- and Cu- Doped Ni-Mn-Ga Alloys. Materials Today: Proceedings, 2015, 2, S601-S604.	0.9	8
32	2D Structures Beyond Graphene. Semiconductors and Semimetals, 2016, 95, 1-33.	0.4	8
33	Coupling between the $4f$ core binding energy and the $5f$ valence band occupation of elemental Pu and Pu-based compounds. Physical Review B, 2008, 78, .	1.1	7
34	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
35	Effects of electron beam generated lattice defects on the periodic lattice distortion structure in S_2 and S_4	1.1	7
36	Launching the Theoretical Crystallography Open Database. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1736-C1736.	0.0	6

#	ARTICLE	IF	CITATIONS
37	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
38	Theoretical studies of the incommensurate magnetic structure of a heavy fermion system: CeRhIn5. Physical Review B, 2010, 81, .	1.1	4
39	Realistic first-principles calculations of the magnetocaloric effect: applications to hcp Gd. Materials Research Letters, 2022, 10, 156-162.	4.1	4
40	Effect of Magnetic Ordering on the Stability of Ni-Mn-Ga-Co-Cu Alloys Along the Tetragonal Deformation Path. IEEE Transactions on Magnetics, 2017, 53, 1-6.	1.2	3