David J Singh

List of Publications by Year
in descending order

235 papers	20,613 citations	15504 65 h-index	11939 134 g-index
240 all docs	240 docs citations	240 times ranked	15206 citing authors

#	Article	IF	Citations
1	BoltzTraP. A code for calculating band-structure dependent quantities. Computer Physics Communications, 2006, 175, 67-71.	7.5	4,184
2	Superconductivity at 22 K in Co-Doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BaFe</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>As</mml:mi><mml:mn> Physical Review Letters, 2008, 101, 117004.	7.8	980
3	Planewaves, Pseudopotentials and the LAPW Method. , 1994, , .		904
4	Electronic structure and half-metallic transport in theLa1âˆ’xCaxMnO3system. Physical Review B, 1996, 53, 1146-1160.	3.2	750
5	Light scattering and surface plasmons on small spherical particles. Light: Science and Applications, 2014, 3, e179-e179.	16.6	450
6	On the tuning of electrical and thermal transport in thermoelectrics: an integrated theoryâ€“experiment perspective. Npj Computational Materials, 2016, 2, .	8.7	399
7	Tuning the carrier scattering mechanism to effectively improve the thermoelectric properties. Energy and Environmental Science, 2017, 10, 799-807.	30.8	326
8	Ferromagnetic Spin Fluctuation Induced Superconductivity inSr2RuO4. Physical Review Letters, 1997, 79, 733-736.	7.8	311
9	Electronic structure calculations with the Tran-Blaha modified Becke-Johnson density functional. Physical Review B, 2010, 82, .	3.2	292
10	LuNi2B2C: A novel Ni-based strong-coupling superconductor. Physical Review Letters, 1994, 72, 3702-3705.	7.8	291
11	Skutterudite antimonides: Quasilinear bands and unusual transport. Physical Review B, 1994, 50, 11235-11238.	3.2	272
12	Giant optical anisotropy in a quasi-one-dimensional crystal. Nature Photonics, 2018, 12, 392-396.	31.4	269
13	Manipulation of ionized impurity scattering for achieving high thermoelectric performance in n-type Mg ₃ Sb ₂ -based materials. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10548-10553.	7.1	267
14	Analysis of the thermoelectric properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>n</mml:mi></mml:mrow></mml:math>-type ZnO. Physical Review B, 2011, 83, .	3.2	265
15	Relationship ofSr2RuO4to the superconducting layered cuprates. Physical Review B, 1995, 52, 1358-1361.	3.2	262
16	Doping-dependent thermopower of PbTe from Boltzmann transport calculations. Physical Review B, 2010, 81, .	3.2	259
17	Electronic structure and transport in type-I and type-VIII clathrates containing strontium, barium, and europium. Physical Review B, 2003, 68, .	3.2	251
18	High-temperature thermoelectric performance of heavily doped PbSe. Physical Review B, 2010, 82, .	3.2	243

#	Article	IF	Citations
19	Discovery of ZrCoBi based half Heuslers with high thermoelectric conversion efficiency. Nature Communications, 2018, 9, 2497.	12.8	243
20	Discovery of TaFeSb-based half-Heuslers with high thermoelectric performance. Nature Communications, 2019, 10, 270.	12.8	227
21	Adsorption of Single Li and the Formation of Small Li Clusters on Graphene for the Anode of Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2013, 5, 7793-7797.	8.0	190
22	Connections between the electron-energy-loss spectra, the local electronic structure, and the physical properties of a material: A study of nickel aluminum alloys. Physical Review B, 1998, 57, 8181-8202.	3.2	185
23	Phase-transition temperature suppression to achieve cubic GeTe and high thermoelectric performance by Bi and Mn codoping. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5332-5337.	7.1	183
24	Connecting Thermoelectric Performance and Topological-Insulator Behavior:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Bi</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mi>Te</mml:mi></mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>Se</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Bi</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:msub><mml:mrow><mml:mi>Te</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:mrow></mml:math>. Physical Review Applied, 2015, 3, .	3.8	178
25	Electronic and magnetic properties of the 4d itinerant ferromagnet SrRuO3. Journal of Applied Physics, 1996, 79, 4818.	2.5	176
26	Electronic structure of Ce-filled skutterudites. Physical Review B, 1996, 53, 1103-1108.	3.2	171
27	Noncollinear Intra-atomic Magnetism. Physical Review Letters, 1996, 76, 4420-4423.	7.8	170
28	Electronic, transport, and optical properties of bulk and mono-layer PdSe2. Applied Physics Letters, 2015, 107, .	3.3	170
29	Structure and optical properties of high light output halide scintillators. Physical Review B, 2010, 82, .	3.2	155
30	Bandgap Control via Structural and Chemical Tuning of Transition Metal Perovskite Chalcogenides. Advanced Materials, 2017, 29, 1604733.	21.0	154
31	Importance of non-parabolic band effects in the thermoelectric properties of semiconductors. Scientific Reports, 2013, 3, 3168.	3.3	147
32	Complex Band Structures and Lattice Dynamics of Bi₂Te₃â€Based Compounds and Solid Solutions. Advanced Functional Materials, 2019, 29, 1900677.	14.9	135
33	Recent progress of TMD nanomaterials: phase transitions and applications. Nanoscale, 2020, 12, 1247-1268.	5.6	132
34	High Three-Dimensional Thermoelectric Performance from Low-Dimensional Bands. Physical Review Letters, 2013, 110, 146601.	7.8	131
35	Influence of band structure on the large thermoelectric performance of lanthanum telluride. Physical Review B, 2009, 79, .	3.2	129
36	Thermoelectric properties of AgGaTe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>and related chalcopyrite structure materials. Physical Review B, 2012, 85, .	3.2	118

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37	Strain effects on the band gap and optical properties of perovskite SrSnO3 and BaSnO3. Applied Physics Letters, 2014, 104, .	3.3	108
38	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	8.7	107
39	Structure and energetics of antiferroelectricPbZrO3. Physical Review B, 1995, 52, 12559-12563.	3.2	105
40	Study of the Thermoelectric Properties of Lead Selenide Doped with Boron, Gallium, Indium, or Thallium. Journal of the American Chemical Society, 2012, 134, 17731-17738.	13.7	105
41	Controlling phase transition for single-layer MTe₂ (M = Mo and W): modulation of the potential barrier under strain. Physical Chemistry Chemical Physics, 2016, 18, 4086-4094.	2.8	105
42	Stability and phonons ofKTaO3. Physical Review B, 1996, 53, 176-180.	3.2	103
43	Absence of superconductivity in hole-doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaFe</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> crystals. Physical Review B, 2009, 79, .	3.2	101
44	Electronic fitness function for screening semiconductors as thermoelectric materials. Physical Review Materials, 2017, 1, .	2.4	98
45	Possible coexistence of rotational and ferroelectric lattice distortions in rhombohedralPbZrxTi1â^'xO3. Physical Review B, 2001, 63, .	3.2	93
46	The Electronic Properties of Single-Layer and Multilayer MoS₂ under High Pressure. Journal of Physical Chemistry C, 2015, 119, 10189-10196.	3.1	89
47	Optical properties of ferroelectric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Bi</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2010, 82, .	3.2	86
48	Bismuth and antimony-based oxyhalides and chalcohalides as potential optoelectronic materials. Npj Computational Materials, 2018, 4, .	8.7	86
49	Benefits of Carrier-Pocket Anisotropy to Thermoelectric Performance: The Case of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-Type<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>AgBiSe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Applied, 2015, 3, .	3.8	84
50	Magnetoelectronic effects in pyrochloreTl2Mn2O7: Role of Tl-O covalency. Physical Review B, 1997, 55, 313-316.	3.2	83
51	Thermoelectric properties of AMg₂X₂, AZn₂Sb₂ (A =) Tj ETQq1 1 0.784314 rgBT /O Materials Chemistry A, 2017, 5, 8499-8509.	10.3	83
52	Unusual Transport and Strongly Anisotropic Thermopower in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>PtCoO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>PdCoO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2010, 104, 176601.	7.8	82
53	Density functional study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaNi</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Electronic structure, phonons, and electron-phonon superconductivity. Physical Review B, 2008, 78, .	3.2	81
54	Seebeck and Figure of Merit Enhancement in Nanostructured Antimony Telluride by Antisite Defect Suppression through Sulfur Doping. Nano Letters, 2012, 12, 4523-4529.	9.1	80

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55	Electronic structure and thermoelectric prospects of phosphide skutterudites. Physical Review B, 1999, 59, 9722-9724.	3.2	76
56	Thermoelectric transport properties of CaMg<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>, EuMg<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	3.2	75
57	Structure and Properties of Single Crystalline CaMg₂Bi₂, EuMg₂Bi₂, and YbMg₂Bi₂. Inorganic Chemistry, 2011, 50, 11127-11133.	4.0	74
58	Valence Band Splitting on Multilayer MoS₂: Mixing of Spinâ€“Orbit Coupling and Interlayer Coupling. Journal of Physical Chemistry Letters, 2016, 7, 2175-2181.	4.6	73
59	Enhanced Born charge and proximity to ferroelectricity in thallium halides. Physical Review B, 2010, 81, .	3.2	72
60	Optical properties of PbTe and PbSe. Physical Review B, 2012, 85, .	3.2	72
61	Experimental Identification of Critical Condition for Drastically Enhancing Thermoelectric Power Factor of Two-Dimensional Layered Materials. Nano Letters, 2018, 18, 7538-7545.	9.1	72
62	High-Throughput Screening for Advanced Thermoelectric Materials: Diamond-Like ABX₂ Compounds. ACS Applied Materials & Interfaces, 2019, 11, 24859-24866.	8.0	72
63	Dimensionality Controlled Octahedral Symmetry-Mismatch and Functionalities in Epitaxial LaCoO₃/SrTiO₃ Heterostructures. Nano Letters, 2015, 15, 4677-4684.	9.1	71
64	Thermoelectric properties of n-type SrTiO3. APL Materials, 2016, 4, .	5.1	71
65	Dielectric Behavior as a Screen in Rational Searches for Electronic Materials: Metal Pnictide Sulfosalts. Journal of the American Chemical Society, 2018, 140, 18058-18065.	13.7	69
66	Elastic instability of bcc cobalt. Physical Review B, 1993, 47, 8515-8519.	3.2	68
67	Achieving band convergence by tuning the bonding ionicity in nâ€type Mg₃Sb₂. Journal of Computational Chemistry, 2019, 40, 1693-1700.	3.3	68
68	Transparent conducting properties of SrSnO₃ and ZnSnO₃. APL Materials, 2015, 3, 062505.	5.1	65
69	Unconventional Oxygen Doping Behavior inHgBa2Ca2Cu3O8+Î´. Physical Review Letters, 1994, 73, 476-479.	7.8	62
70	Adsorption of Li on single-layer silicene for anodes of Li-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 8887-8896.	2.8	62
71	Heavy element doping for enhancing thermoelectric properties of nanostructured zinc oxide. RSC Advances, 2014, 4, 6363.	3.6	61
72	Electronic characteristics of Tl2Ba2CuO6. Physica C: Superconductivity and Its Applications, 1992, 203, 193-202.	1.2	60

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73	Local density and generalized gradient approximation studies of KNbO3 and BaTiO3. Ferroelectrics, 1995, 164, 143-152.	0.6	58
74	Spin glass and semiconducting behavior in one-dimensional BaFe2â˜Î´Se3(Î´â‰ˆ0.2)crystals. Physical Review B, 2011, 84, .	3.2	58
75	Electronic structure and energetics of the tetragonal distortion for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiH</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu	3.2	57
76	Electronic structure and thermoelectric properties:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbBi</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms related intergrowth compounds. Physical Review B, 2010, 81, .	3.2	56
77	Nanostructuring and more. Nature Materials, 2008, 7, 616-617.	27.5	55
78	TransOpt. A code to solve electrical transport properties of semiconductors in constant electronâ€“phonon coupling approximation. Computational Materials Science, 2021, 186, 110074.	3.0	55
79	Understanding the asymmetrical thermoelectric performance for discovering promising thermoelectric materials. Science Advances, 2019, 5, eaav5813.	10.3	52
80	Magnetic and electronic properties ofLiMnO2s. Physical Review B, 1997, 55, 309-312.	3.2	51
81	THERMOPOWER OF SnTe FROM BOLTZMANN TRANSPORT CALCULATIONS. Functional Materials Letters, 2010, 03, 223-226.	1.2	50
82	Electronic structure of HgBa2CuO4. Physica C: Superconductivity and Its Applications, 1993, 212, 228-232.	1.2	49
83	Optimal Bandgap in a 2D Ruddlesdenâ€“Popper Perovskite Chalcogenide for Single-Junction Solar Cells. Chemistry of Materials, 2018, 30, 4882-4886.	6.7	49
84	Chapter 5 Theoretical and computational approaches for identifying and optimizing novel thermoelectric materials. Semiconductors and Semimetals, 2001, , 125-177.	0.7	48
85	Potential thermoelectric performance of hole-doped Cu₂O. New Journal of Physics, 2013, 15, 043029.	2.9	47
86	Dynamic Optical Tuning of Interlayer Interactions in the Transition Metal Dichalcogenides. Nano Letters, 2017, 17, 7761-7766.	9.1	46
87	Modulation of Hydrogen Evolution Catalytic Activity of Basal Plane in Monolayer Platinum and Palladium Dichalcogenides. ACS Omega, 2018, 3, 10058-10065.	3.5	46
88	Layered Tl₂O: a model thermoelectric material. Journal of Materials Chemistry C, 2019, 7, 5094-5103.	5.5	46
89	Electronic and thermoelectric properties of CoSbS and FeSbS. Physical Review B, 2013, 87, .	3.2	45
90	Electronic and transport properties of zintl phase AeMg2Pn2, Aeâ€‰=â€‰Ca,Sr,Ba, Pnâ€‰=â€‰As,Sb,Bi in relation to Mg3Sb2. Journal of Applied Physics, 2013, 114, 143703.	2.5	45

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91	Thermoelectric Properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>Mg</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:mi>Ge</mml:mi><mml:mo>,</mml:mo><mml:mi>Sn</mml:mi><mml:mo stretchy="false">)</mml:mo></mml:mrow></mml:mrow></mml:math>. Physical Review Applied, 2016, 5, .	3.8	45
92	Harnessing Topological Band Effects in Bismuth Telluride Selenide for Large Enhancements in Thermoelectric Properties through Isovalent Doping. Advanced Materials, 2016, 28, 6436-6441.	21.0	44
93	Optic phonons and anisotropic thermal conductivity in hexagonal Ge2Sb2Te5. Scientific Reports, 2016, 6, 37076.	3.3	44
94	n-Type TaCoSn-Based Half-Heuslers as Promising Thermoelectric Materials. ACS Applied Materials & Interfaces, 2019, 11, 41321-41329.	8.0	44
95	Electronic structure, localization, and spin-state transition in Cu-substituted<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>FeSe</mml:mtext><mml:mo>:</mml:mo><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow> Physical Review B, 2010, 81, .	3.2	43
96	Transport, thermal, and magnetic properties of the narrow-gap semiconductor CrSb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	3.2	43
97	Perspective: n-type oxide thermoelectrics via visual search strategies. APL Materials, 2016, 4, .	5.1	42
98	Adsorption and Formation of Small Na Clusters on Pristine and Double-Vacancy Graphene for Anodes of Na-Ion Batteries. ACS Applied Materials & Interfaces, 2017, 9, 17076-17084.	8.0	42
99	Computational modelling of the thermoelectric properties of p-type Zintl compound CaMg2Bi2. Materials Today Physics, 2017, 2, 40-45.	6.0	40
100	Thermoelectric properties of p-type cubic and rhombohedral GeTe. Journal of Applied Physics, 2018, 123, .	2.5	40
101	Thermoelectric Properties of Zintl Phase YbMg₂Sb₂. Chemistry of Materials, 2020, 32, 776-784.	6.7	40
102	First principles study on 2Hâ€“1Tâ€² transition in MoS₂ with copper. Physical Chemistry Chemical Physics, 2018, 20, 26986-26994.	2.8	39
103	Antiferromagnetism in a Technetium Oxide. Structure of CaTcO₃. Journal of the American Chemical Society, 2011, 133, 1654-1657.	13.7	38
104	Pressure evolution of the potential barriers of phase transition of MoS₂, MoSe₂ and MoTe₂. Physical Chemistry Chemical Physics, 2016, 18, 12080-12085.	2.8	38
105	bcc cobalt: Metastable phase or forced structure?. Journal of Applied Physics, 1993, 73, 6189-6191.	2.5	37
106	Prospective high thermoelectric performance of the heavily <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="bold-italic">p</mml:mi></mml:math> -doped half-Heusler compound CoVSn. Physical Review B, 2017, 95, .	3.2	37
107	General-potential study of the electronic and magnetic structure of FeCo. Physical Review B, 1992, 46, 11145-11148.	3.2	36
108	Suppression of spin density wave by isoelectronic substitution in. Journal of Solid State Chemistry, 2009, 182, 2326-2331.	2.9	36

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109	Potential Thermoelectric Performance from Optimization of Hole-Doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Se</mml:mi><mml:mn	8.9	36
110	Electronic structure, transport, and phonons of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrAg</mml:mi><mml:mi>C</mml:mi><mml:mi>h</mml:mi><mml:mathvariant="normal">F</mml:mi></mml:mrow></mml:math>(<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 702 Td (xmlns:mml="	3.2	36
111	Electronic Properties, Screening, and Efficient Carrier Transport in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NaSbS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn>	3.8	36
112	The thermal and thermoelectric transport properties of SiSb, GeSb and SnSb monolayers. Journal of Materials Chemistry C, 2019, 7, 10652-10662.	5.5	36
113	BaT2As2 single crystals (T=Fe, Co, Ni) and superconductivity upon Co-doping. Physica C: Superconductivity and Its Applications, 2009, 469, 350-354.	1.2	35
114	Chemistry and electronic structure of iron-based superconductors. MRS Bulletin, 2011, 36, 614-619.	3.5	35
115	Competing covalent and ionic bonding in Ge-Sb-Te phase change materials. Scientific Reports, 2016, 6, 25981.	3.3	35
116	Adsorption of Na on silicene for potential anode for Na-ion batteries. Electrochimica Acta, 2019, 297, 497-503.	5.2	35
117	Electronic structure ofHgBa2Ca2Cu3O8: The role of mercury. Physical Review B, 1993, 48, 3571-3574.	3.2	34
118	Electron-phonon superconductivity in noncentrosymmetricLaNiC2: First-principles calculations. Physical Review B, 2009, 80, .	3.2	34
119	Properties of alkaline-earth-filled skutterudite antimonides:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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127	Tuning optical properties of transparent conducting barium stannate by dimensional reduction. APL Materials, 2015, 3, .	5.1	29
128	Complex doping of group 13 elements In and Ga in caged skutterudite CoSb3. Acta Materialia, 2015, 85, 112-121.	7.9	29
129	Design of ternary alkaline-earth metal Sn(<scp>ii</scp>) oxides with potential good p-type conductivity. Journal of Materials Chemistry C, 2016, 4, 4592-4599.	5.5	29
130	Density functional studies of PbZrO3, KTaO3and KNbO3. Ferroelectrics, 1997, 194, 299-322.	0.6	28
131	Electronic structure and lattice distortions inPbMg1âˆ•3Nb2âˆ•3O3studied with density functional theory using the linearized augmented plane-wave method. Physical Review B, 2006, 73, .	3.2	28
132	Metallic nickel silicides: Experiments and theory for NiSi and first principles calculations for other phases. Journal of Alloys and Compounds, 2016, 672, 110-116.	5.5	28
133	Weighted-density-approximation ground-state studies of solids. Physical Review B, 1993, 48, 14099-14103.	3.2	27
134	Crystal, magnetic and electronic structures and properties of new BaMnPnF (Pn = As, Sb, Bi). Scientific Reports, 2013, 3, 2154.	3.3	27
135	Electronic structure ofPrBa2Cu3O7. Physical Review B, 1994, 50, 4106-4111.	3.2	26
136	Electronic and structural properties ofLa3Ni2B2N3. Physical Review B, 1995, 51, 8668-8671.	3.2	26
137	LaPt2B2C: A conventional borocarbide superconductor. Physical Review B, 1994, 50, 6486-6488.	3.2	25
138	Transport and optical properties of heavily hole-doped semiconductors BaCu2Se2 and BaCu2Te2. Journal of Solid State Chemistry, 2011, 184, 2744-2750.	2.9	25
139	Itinerant origin of the ferromagnetic quantum critical point in Fe(Ga,Ge)3. Physical Review B, 2013, 88, .	3.2	25
140	Zintl chemistry leading to ultralow thermal conductivity, semiconducting behavior, and high thermoelectric performance of hexagonal KBaBi. Physical Review B, 2021, 103, .	3.2	24
141	Thermoelectric properties of Î²-FeSi2. Journal of Applied Physics, 2013, 114, .	2.5	23
142	Electronic structure and the origin of the high ordering temperature in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SrRu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>6</mml:mn></mml:mrow></mml:math>. Physical Review B, 2015, 91, .	3.2	23
143	Modulation of electronic properties from stacking orders and spin-orbit coupling for 3R-type MoS2. Scientific Reports, 2016, 6, 24140.	3.3	23
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