David Joseph Singh

List of Publications by Year
in descending order

355 papers	51,865 citations	5876 81 h-index	1341 223 g-index
363 all docs	363 docs citations	363 times ranked	32456 citing authors

#	Article	IF	Citations
1	Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. Physical Review B, 1992, 46, 6671-6687.	1.1	19,217
2	BoltzTraP. A code for calculating band-structure dependent quantities. Computer Physics Communications, 2006, 175, 67-71.	3.0	4,184
3	Unconventional Superconductivity with a Sign Reversal in the Order Parameter of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LaFeAsO</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math> mathvariant="normal">F</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>. Physical Review	2.9	2,270
4	Density Functional Study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LaFeAsO</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math> mathvariant="normal">F</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>: A Low Carrier Density Superconductor Near Itinerant Magnetism. Physical Review Letters, 2008, 100, 237003.	2.9	1,049
5	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:msub> Physical Review Letters, 2008, 101, 117004.	2.9	980
6	Electronic structure and half-metallic transport in theLa1â^'xCaxMnO3system. Physical Review B, 1996, 53, 1146-1160.	1.1	750
7	Giant anharmonic phonon scattering in PbTe. Nature Materials, 2011, 10, 614-619.	13.3	561
8	Light scattering and surface plasmons on small spherical particles. Light: Science and Applications, 2014, 3, e179-e179.	7.7	450
9	On the tuning of electrical and thermal transport in thermoelectrics: an integrated theoryâ€"experiment perspective. Npj Computational Materials, 2016, 2, .	3.5	399
10	Electronic structure and magnetism in Ru-based perovskites. Physical Review B, 1997, 56, 2556-2571.	1.1	377
11	Problems with reconciling density functional theory calculations with experiment in ferropnictides. Physical Review B, 2008, 78, .	1.1	352
12	Tuning the carrier scattering mechanism to effectively improve the thermoelectric properties. Energy and Environmental Science, 2017, 10, 799-807.	15.6	326
13	Electronic correlations in the iron pnictides. Nature Physics, 2009, 5, 647-650.	6.5	317
14	Ferromagnetic Spin Fluctuation Induced Superconductivity inSr2RuO4. Physical Review Letters, 1997, 79, 733-736.	2.9	311
15	Electronic structure calculations with the Tran-Blaha modified Becke-Johnson density functional. Physical Review B, 2010, 82, .	1.1	292
16	Calculated thermoelectric properties of La-filled skutterudites. Physical Review B, 1997, 56, R1650-R1653.	1.1	283
17	Electronic structure of the iron-based superconductor LaOFeP. Nature, 2008, 455, 81-84.	13.7	279
18	Giant optical anisotropy in a quasi-one-dimensional crystal. Nature Photonics, 2018, 12, 392-396.	15.6	269

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19	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.	3.3	267
20	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, .	1.1	265
21	Relationship ofSr2RuO4to the superconducting layered cuprates. Physical Review B, 1995, 52, 1358-1361.	1.1	262
22	Doping-dependent thermopower of PbTe from Boltzmann transport calculations. Physical Review B, 2010, 81, .	1.1	259
23	Electronic structure and transport in type-I and type-VIII clathrates containing strontium, barium, and europium. Physical Review B, 2003, 68, .	1.1	251
24	High-temperature thermoelectric performance of heavily doped PbSe. Physical Review B, 2010, 82, .	1.1	243
25	Discovery of ZrCoBi based half Heuslers with high thermoelectric conversion efficiency. Nature Communications, 2018, 9, 2497.	5.8	243
26	Wide bandgap tunability in complex transition metal oxides by site-specific substitution. Nature Communications, 2012, 3, 689.	5.8	237
27	Competitions in Layered Ruthenates: Ferromagnetism versus Antiferromagnetism and Triplet versus Singlet Pairing. Physical Review Letters, 1999, 82, 4324-4327.	2.9	229
28	Discovery of TaFeSb-based half-Heuslers with high thermoelectric performance. Nature Communications, 2019, 10, 270.	5.8	227
29	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.	4.0	190
30	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.	3.3	183
31	Room-temperature intrinsic ferromagnetism in epitaxial CrTe2 ultrathin films. Nature Communications, 2021, 12, 2492.	5.8	179
32	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:msub><mml:mrow><mml:mi>Te</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></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:msub><mml:mrow><mml:mi>Se</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review Applied, 2015, 3, .	1.5	178
33	Electronic and magnetic properties of the 4d itinerant ferromagnet SrRuO3. Journal of Applied Physics, 1996, 79, 4818.	1.1	176
34	Electronic, transport, and optical properties of bulk and mono-layer PdSe2. Applied Physics Letters, 2015, 107, .	1.5	170
35	Gradient-corrected density functionals: Full-potential calculations for iron. Physical Review B, 1991, 43, 11628-11634.	1.1	166
36	Chemical bonding, conductive network, and thermoelectric performance of the ternary semiconductors Cu<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>Sn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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37	Structure and optical properties of high light output halide scintillators. Physical Review B, 2010, 82, .	1.1	155
38	Bandgap Control via Structural and Chemical Tuning of Transition Metal Perovskite Chalcogenides. Advanced Materials, 2017, 29, 1604733.	11.1	154
39	Hydrogen Stabilized RhPdH 2D Bimetallene Nanosheets for Efficient Alkaline Hydrogen Evolution. Journal of the American Chemical Society, 2020, 142, 3645-3651.	6.6	152
40	Importance of non-parabolic band effects in the thermoelectric properties of semiconductors. Scientific Reports, 2013, 3, 3168.	1.6	147
41	Quantum critical behavior and possible triplet superconductivity in electron-dopedCoO2sheets. Physical Review B, 2003, 68, .	1.1	136
42	Complex Band Structures and Lattice Dynamics of Bi₂Te₃â€Based Compounds and Solid Solutions. Advanced Functional Materials, 2019, 29, 1900677.	7.8	135
43	Unconventional electronic reconstruction in undoped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mtext>Ba</mml:mtext><mml:mo>,</mml:mo> the spin density wave transition. Physical Review B, 2009, 80, .	1.1	134
44	Recent progress of TMD nanomaterials: phase transitions and applications. Nanoscale, 2020, 12, 1247-1268.	2.8	132
45	High Three-Dimensional Thermoelectric Performance from Low-Dimensional Bands. Physical Review Letters, 2013, 110, 146601.	2.9	131
46	Influence of band structure on the large thermoelectric performance of lanthanum telluride. Physical Review B, 2009, 79, .	1.1	129
47	Doping and temperature dependence of thermoelectric properties in Mg2(Si,Sn). Physical Review B, 2012, 86, .	1.1	126
48	Phonon Self-Energy and Origin of Anomalous Neutron Scattering Spectra in SnTe and PbTe Thermoelectrics. Physical Review Letters, 2014, 112, 175501.	2.9	125
49	First-principles mode-by-mode analysis for electron-phonon scattering channels and mean free path spectra in GaAs. Physical Review B, 2017, 95, .	1.1	125
50	First principles analysis of vibrational modes in KNbO3. Ferroelectrics, 1992, 136, 95-103.	0.3	121
51	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, .	1.1	118
52	Applicability of the Strongly Constrained and Appropriately Normed Density Functional to Transition-Metal Magnetism. Physical Review Letters, 2018, 121, 207201.	2.9	118
53	Lattice dynamics and reduced thermal conductivity of filled skutterudites. Physical Review B, 2000, 61, R9209-R9212.	1.1	116
54	Electronic structure of the<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:mn>2</mml:mn> of iron-pnictide superconductors. Physical Review B, 2009, 80, .	1.1	116

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55	Suppression of thermopower of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Na</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi mathvariant="normal">Co</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> by an electronic structure and magnetism in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaMn</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m	1.1	114
56	xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaMn</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m Physical Review B, 2009, 79, .	1.1	112
57	Large thermoelectric power factor from crystal symmetry-protected non-bonding orbital in half-Heuslers. Nature Communications, 2018, 9, 1721.	5.8	111
58	Electric-field-gradient calculations for systems with large extended-core-state contributions. Physical Review B, 1992, 46, 1321-1325.	1.1	108
59	Strain effects on the band gap and optical properties of perovskite SrSnO3 and BaSnO3. Applied Physics Letters, 2014, 104, .	1.5	108
60	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	3.5	107
61	Evidence for Strong Itinerant Spin Fluctuations in the Normal State of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CeFeAsO</mml:mi><mml:mn>0.89</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">F</mml:mi><mml:mn>0.11</mml:mn></mml:msub></mml:math>Iron-Oxypnictide Superconductors. Physical Review Letters, 2008, 101, 267001.	2.9	106
62	Favorable Energy Band Alignment of TiO₂ Anatase/Rutile Heterophase Homojunctions Yields Photocatalytic Hydrogen Evolution with Quantum Efficiency Exceeding 45.6%. Advanced Energy Materials, 2022, 12, .	10.2	106
63	First-principles study of the stability of BN and C. Physical Review B, 2001, 64, .	1.1	105
64	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.	1.3	105
65	Theoretical determination that electrons act as anions in the electride Cs+ (15-crown-5)2Â·e-. Nature, 1993, 365, 39-42.	13.7	102
66	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:r crystals. Physical Review B, 2009, 79, .	1.1	101
67	Electronic structure and magnetism ofSr3Ru2O7. Physical Review B, 2001, 63, .	1.1	100
68	High Temperature Magnetic Ordering in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mn>4</mml:mn><mml:mi>d</mml:mi></mml:math>Perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SrTcO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2011, 106, 067201.	2.9	99
69	Electronic fitness function for screening semiconductors as thermoelectric materials. Physical Review Materials, 2017, 1, .	0.9	98
70	Fermi Surface and van Hove Singularities in the Itinerant Metamagnet<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Sr</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi>Ru</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 026407.	2.9	94
71	Second Harmonic Generation Susceptibilities from Symmetry Adapted Wannier Functions. Physical Review Letters, 2020, 125, 187402.	2.9	94
72	Evidence for three-dimensional Fermi-surface topology of the layered electron-doped iron superconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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73	The Electronic Properties of Single-Layer and Multilayer MoS₂ under High Pressure. Journal of Physical Chemistry C, 2015, 119, 10189-10196.	1.5	89
74	Establishing the carrier scattering phase diagram for ZrNiSn-based half-Heusler thermoelectric materials. Nature Communications, 2020, 11, 3142.	5.8	87
75	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> Physical Review B, 2010, 82, .	1.1	86
76	Bismuth and antimony-based oxyhalides and chalcohalides as potential optoelectronic materials. Npj Computational Materials, 2018, 4, .	3.5	86
77	Giant piezoelectricity in oxide thin films with nanopillar structure. Science, 2020, 369, 292-297.	6.0	86
78	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> Physical Review Applied, 2015, 3, .	1.5	84
79	Thermoelectric properties of AMg₂X₂, AZn₂Sb₂ (A =) Tj ETQq1 1 0.784314 rgBT Materials Chemistry A, 2017, 5, 8499-8509.	5.2	83
80	WhyNi3Alls an Itinerant Ferromagnet butNi3Gals Not. Physical Review Letters, 2004, 92, 147201.	2.9	82
81	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.	2.9	82
82	Surface plasmon resonance technique for directly probing the interaction of DNA and graphene oxide and ultra-sensitive biosensing. Biosensors and Bioelectronics, 2014, 58, 374-379.	5.3	81
83	Magnetism and electronic structure of La<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>ZnIrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>and La<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	1.1	80
84	Orbital controlled band gap engineering of tetragonal BiFeO₃ for optoelectronic applications. Journal of Materials Chemistry C, 2018, 6, 1239-1247.	2.7	80
85	Electronic and thermoelectric properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Cu</mml:mi><mml:mi mathvariant="normal">Co</mml:mi><mml:msub><mml:mi	1.1	75
86	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 />	1.1	75
87	Structure and Properties of Single Crystalline CaMg₂Bi₂, EuMg₂Bi₂, and YbMg₂Bi₂. Inorganic Chemistry, 2011, 50, 11127-11133.	1.9	74
88	Valence Band Splitting on Multilayer MoS₂: Mixing of Spinâ€“Orbit Coupling and Interlayer Coupling. Journal of Physical Chemistry Letters, 2016, 7, 2175-2181.	2.1	73
89	Enhanced Born charge and proximity to ferroelectricity in thallium halides. Physical Review B, 2010, 81, .	1.1	72
90	Optical properties of PbTe and PbSe. Physical Review B, 2012, 85, .	1.1	72

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91	Experimental Identification of Critical Condition for Drastically Enhancing Thermoelectric Power Factor of Two-Dimensional Layered Materials. Nano Letters, 2018, 18, 7538-7545.	4.5	72
92	High-Throughput Screening for Advanced Thermoelectric Materials: Diamond-Like ABX₂ Compounds. ACS Applied Materials & Interfaces, 2019, 11, 24859-24866.	4.0	72
93	Dimensionality Controlled Octahedral Symmetry-Mismatch and Functionalities in Epitaxial LaCoO₃/SrTiO₃ Heterostructures. Nano Letters, 2015, 15, 4677-4684.	4.5	71
94	Thermoelectric properties of n-type SrTiO3. APL Materials, 2016, 4, .	2.2	71
95	Dielectric Behavior as a Screen in Rational Searches for Electronic Materials: Metal Pnictide Sulfosalts. Journal of the American Chemical Society, 2018, 140, 18058-18065.	6.6	69
96	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. Chemistry of Materials, 2016, 28, 1746-1755.	3.2	68
97	Achieving band convergence by tuning the bonding ionicity in nâ€type Mg₃Sb₂. Journal of Computational Chemistry, 2019, 40, 1693-1700.	1.5	68
98	Zintl-phase compounds with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnSb</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> anions: Electronic structure and thermoelectric properties. Physical Review B, 2010, 81, .	4.1	66
99	Wet-chemistry hydrogen doped TiO2 with switchable defects control for photocatalytic hydrogen evolution. Matter, 2022, 5, 206-218.	5.0	66
100	Transparent conducting properties of SrSnO₃ and ZnSnO₃. APL Materials, 2015, 3, 062505.	2.2	65
101	High- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:mrow></mml:math> Superconductivity in FeSe at High Pressure: Dominant Hole Carriers and Enhanced Spin Fluctuations. Physical Review Letters, 2017, 118, 147004.	2.9	64
102	Origin of the phase transition in IrTe<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>: Structural modulation and local bonding instability. Physical Review B, 2013, 88, .	1.1	62
103	Ferromagnetism of Fe3Sn and Alloys. Scientific Reports, 2014, 4, 7024.	1.6	62
104	Adsorption of Li on single-layer silicene for anodes of Li-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 8887-8896.	1.3	62
105	Heavy element doping for enhancing thermoelectric properties of nanostructured zinc oxide. RSC Advances, 2014, 4, 6363.	1.7	61
106	Reemergence of high-Tc superconductivity in the (Li1-xFe x)OHFe1-ySe under high pressure. Nature Communications, 2018, 9, 380.	5.8	60
107	Boronâ€“oxygen complex yields n-type surface layer in semiconducting diamond. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7703-7711.	3.3	60
108	Bottom-up growth of homogeneous MoirÃ© superlattices in bismuth oxychloride spiral nanosheets. Nature Communications, 2019, 10, 4472.	5.8	59

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109	Local density and generalized gradient approximation studies of KNbO3 and BaTiO3. Ferroelectrics, 1995, 164, 143-152.	0.3	58
110	Spin glass and semiconducting behavior in one-dimensional BaFe2â˜Î˙Se3(Î˙â‰ˆ0.2)crystals. Physical Review B, 2011, 84, .	1.1	58
111	Magnetic order and electronic structure of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>5</mml:mn><mml:msup><mml:mi>d</mml:mi><mml:mn> perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:mn> Physical Review B, 2015, 91, .	1.1	58
112	Electronic structure of Ba(Sn,Sb)O3: Absence of superconductivity. Physical Review B, 1991, 44, 9519-9523.	1.1	57
113	Electronic structure and thermoelectric properties of layered<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbSe-WSe</mml:mtext></mml:mrow><mml:mn>2</mml:mn><mml:mn> Physical Review B, 2009, 80, .	1.1	57
114	Atomically Dispersed MoO_x on Rhodium Metallene Boosts Electrocatalyzed Alkaline Hydrogen Evolution. Angewandte Chemie - International Edition, 2022, 61, .	7.2	57
115	TransOpt. A code to solve electrical transport properties of semiconductors in constant electronâ€“phonon coupling approximation. Computational Materials Science, 2021, 186, 110074.	1.4	55
116	Low-Temperature Magnetothermal Transport Investigation of a Ni-Based Superconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BaNi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>As</mml:mi><mml:mi><mml:n Evidence for Fully Gapped Superconductivity. Physical Review Letters, 2009, 102, 147004.	2.9	54
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