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	Computational search for itinerant <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -type and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -type magnetic semiconductors: Arsenopyrites as bipolar magnetic semiconductors. Physical Review B, 2022, 105, .	3.2	0
2	Low thermal conductivity and high thermoelectric performance via Cd underbonding in half-Heusler PCdNa. Physical Review B, 2022, 105, .	3.2	15
3	Complex structure due to As bonding and interplay with electronic structure in superconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>BaNi</mml:mi><mml:mn>2</mml:mn></m Physical Review B, 2022, 105, .	3.2	5
4	Unraveling the relationships between chemical bonding and thermoelectric properties: n-type ABO₃ perovskites. Journal of Materials Chemistry A, 2022, 10, 11039-11045.	10.3	10
5	Designing Rashba systems for high thermoelectric performance based on the van der Waals heterostructure. Materials Today Physics, 2022, 27, 100788.	6.0	1
6	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
7	Vertical Strain Engineering of Epitaxial La 2/3 Sr 1/3 MnO 3 Thin Films by Spontaneously Embedding ZrO 2 Nanopillar Arrays. Advanced Materials Interfaces, 2021, 8, 2001355.	3.7	1
8	Disorder and Itinerant Magnetism in Full Heusler Pd2TiIn. Chinese Physics Letters, 2021, 38, 017102.	3.3	1
9	Storage mechanism of K in hydrogen-substituted graphdiyne as a superior anode. Journal of Materials Chemistry A, 2021, 9, 12320-12330.	10.3	4
10	Improved thermoelectric transport properties of Ge₄Se₃Te through dimensionality reduction. Journal of Materials Chemistry C, 2021, 9, 1804-1813.	5.5	17
11	Binary and Ternary Colloidal Cuâ€Snâ€Te Nanocrystals for Thermoelectric Thin Films. Small, 2021, 17, e2006729.	10.0	8
12	Vacancy ordering induced topological electronic transition in bulk Eu ₂ ZnSb ₂. Science Advances, 2021, 7, .	10.3	21
13	Multigap electron-phonon superconductivity in the quasi-one-dimensional pnictide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">K</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Mo</mml:mi><mml:mn>3</mml:mn></m Physical Review B, 2021, 103, .	3.2	4
14	Ferromagnetism in a Semiconductor with Mobile Carriers via Low-Level Nonmagnetic Doping. Physical Review Applied, 2021, 15, .	3.8	3
15	Zintl chemistry leading to ultralow thermal conductivity, semiconducting behavior, and high thermoelectric performance of hexagonal KBaBi. Physical Review B, 2021, 103, .	3.2	24
16	Thermoelectrics by Computational Design: Progress and Opportunities. Annual Review of Materials Research, 2021, 51, 565-590.	9.3	23
17	Adsorption of K Ions on Single-Layer GeC for Potential Anode of K Ion Batteries. Nanomaterials, 2021, 11, 1900.	4.1	6
18	Thermoelectric Properties of Zintl Phase YbMg₂Sb₂. Chemistry of Materials, 2020, 32, 776-784.	6.7	40

#	Article	IF	Citations
19	Recent progress of TMD nanomaterials: phase transitions and applications. Nanoscale, 2020, 12, 1247-1268.	5.6	132
20	Ultralow Thermal Conductivity in Csâ€“Sbâ€“Se Compounds: Lattice Instability versus Lone-Pair Electrons. Chemistry of Materials, 2020, 32, 8906-8913.	6.7	18
21	Copper(I)-Based Flexible Organicâ€“Inorganic Coordination Polymer and Analogues: High-Power Factor Thermoelectrics. ACS Applied Materials & Interfaces, 2020, 12, 53841-53851.	8.0	14
22	Competing magnetic orders in quantum critical <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Sr</mml:mi></mml:mrow><mml:mn>3</mml:mn> mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>7</mml:mn></mml:msub></mml:math>. Physical Review B, 2020, 102, .	3.2	5
23	Enhanced Thermoelectric Performance in Black Phosphorus Nanotubes by Band Modulation through Tailoring Nanotube Chirality. Small, 2020, 16, e2001820.	10.0	13
24	Thermoelectric properties of monolayer GeAsSe and SnSbTe. Journal of Materials Chemistry C, 2020, 8, 9763-9774.	5.5	22
25	Electronic and magnetic properties of perovskite selenite and tellurite compounds: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CoSeO</mml:mi><mml:mn>3</mml:mn></mml:msub><m , and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NiTeO</mml:mi><mml:mn>. Physical Review B, 2020, 101, .	3.2	11
26	Achieving high-performance p-type SmMg₂Bi₂ thermoelectric materials through band engineering and alloying effects. Journal of Materials Chemistry A, 2020, 8, 15760-15766.	10.3	21
27	Quantum critical point and ferromagnetic semiconducting behavior in p -type FeAs2. Physical Review B, 2020, 101, .	3.2	5
28	Defect Engineering for Realizing p-Type AgBiSe₂ with a Promising Thermoelectric Performance. Chemistry of Materials, 2020, 32, 3528-3536.	6.7	17
29	Interplay of local moment and itinerant magnetism in cobalt-based Heusler ferromagnets: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml:mn>2</mml:mn></mml:mr and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml:mn>2</mml:mn></mml:m. Physical Review B, 2020, 101, .	3.2	17
30	Prediction of ternary alkaline-earth metal Sn(II) and Pb(II) chalcogenide semiconductors. Physical Review Materials, 2020, 4, .	2.4	1
31	The thermal and thermoelectric transport properties of SiSb, GeSb and SnSb monolayers. Journal of Materials Chemistry C, 2019, 7, 10652-10662.	5.5	36
32	Electronic structure as a guide in screening for potential thermoelectrics: Demonstration for half-Heusler compounds. Physical Review B, 2019, 100, .	3.2	34
33	n-Type TaCoSn-Based Half-Heuslers as Promising Thermoelectric Materials. ACS Applied Materials & Interfaces, 2019, 11, 41321-41329.	8.0	44
34	3D Printing of Solutionâ€Processable 2D Nanoplates and 1D Nanorods for Flexible Thermoelectrics with Ultrahigh Power Factor at Lowâ€Medium Temperatures. Advanced Science, 2019, 6, 1901788.	11.2	33
35	Understanding the asymmetrical thermoelectric performance for discovering promising thermoelectric materials. Science Advances, 2019, 5, eaav5813.	10.3	52
36	Structural instability and magnetism of superconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>KCr</mml:mi><mml:mn>2</mml:mn></mml:m Physical Review B, 2019, 99, .	3.2	11

#	Article	IF	Citations
37	Doping dependence of the magnitude of fluctuating spin moments in the normal state of the pnictide superconductor Sr(Fe1â^'xCox)2As2 inferred from photoemission spectroscopy. Physical Review B, 2019, 99, .	3.2	0
38	Complex Band Structures and Lattice Dynamics of Bi₂Te₃â€Based Compounds and Solid Solutions. Advanced Functional Materials, 2019, 29, 1900677.	14.9	135
39	High-Throughput Screening for Advanced Thermoelectric Materials: Diamond-Like ABX₂ Compounds. ACS Applied Materials & Interfaces, 2019, 11, 24859-24866.	8.0	72
40	Divalent doping-induced thermoelectric power factor increase in p-type Bi2Te3 via electronic structure tuning. Journal of Applied Physics, 2019, 125, .	2.5	11
41	Achieving band convergence by tuning the bonding ionicity in nâ€type Mg₃Sb₂. Journal of Computational Chemistry, 2019, 40, 1693-1700.	3.3	68
42	Layered Tl₂O: a model thermoelectric material. Journal of Materials Chemistry C, 2019, 7, 5094-5103.	5.5	46
43	Storage of Na in layered graphdiyne as high capacity anode materials for sodium ion batteries. Journal of Materials Chemistry A, 2019, 7, 25609-25618.	10.3	20
44	Tuning from frustrated magnetism to superconductivity in quasi-one-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>KCr</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> through hydrogen doping. Physical Review B, 2019, 100, .	3.2	15
45	Discovery of TaFeSb-based half-Heuslers with high thermoelectric performance. Nature Communications, 2019, 10, 270.	12.8	227
46	Adsorption of Na on silicene for potential anode for Na-ion batteries. Electrochimica Acta, 2019, 297, 497-503.	5.2	35
47	First principles based screen for identification of transparent conductors. Journal of Materials Chemistry C, 2019, 7, 2436-2442.	5.5	5
48	Adsorption of Li on single-layer silicene for anodes of Li-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 8887-8896.	2.8	62
49	Thermoelectric properties of layered NaSbSe₂. Journal of Physics Condensed Matter, 2018, 30, 225501.	1.8	10
50	Synthesis and Crystal Structure of the Layered Lanthanide Oxychlorides Ba₃Ln₂O₅Cl₂. Inorganic Chemistry, 2018, 57, 1727-1734.	4.0	9
51	Bismuth and antimony-based oxyhalides and chalcohalides as potential optoelectronic materials. Npj Computational Materials, 2018, 4, .	8.7	86
52	Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures. MRS Advances, 2018, 3, 397-402.	0.9	5
53	First principles study on 2Hâ€“1Tâ€² transition in MoS₂ with copper. Physical Chemistry Chemical Physics, 2018, 20, 26986-26994.	2.8	39
54	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

#	Article	IF	Citations
55	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	8.7	107
56	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
57	Frustrated Structural Instability in Superconducting Quasi-One-Dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">K</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow><mm Physical Review Letters, 2018, 121, 137002.	7.8	16
58	Modulation of Hydrogen Evolution Catalytic Activity of Basal Plane in Monolayer Platinum and Palladium Dichalcogenides. ACS Omega, 2018, 3, 10058-10065.	3.5	46
59	Thermoelectric properties of p-type cubic and rhombohedral GeTe. Journal of Applied Physics, 2018, 123, .	2.5	40
60	Optimal Bandgap in a 2D Ruddlesdenâ€“Popper Perovskite Chalcogenide for Single-Junction Solar Cells. Chemistry of Materials, 2018, 30, 4882-4886.	6.7	49
61	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
62	Tunability of electronic and optical properties of the Baâ€“Zrâ€“S system via dimensional reduction. European Physical Journal B, 2018, 91, 1.	1.5	16
63	Giant optical anisotropy in a quasi-one-dimensional crystal. Nature Photonics, 2018, 12, 392-396.	31.4	269
64	Discovery of ZrCoBi based half Heuslers with high thermoelectric conversion efficiency. Nature Communications, 2018, 9, 2497.	12.8	243
65	Optical and electronic properties of doped p -type CuI: Explanation of transparent conductivity from first principles. Physical Review Materials, 2018, 2, .	2.4	7
66	Thermal conductivity of perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>KTaO</mml:mi><mml:mn>3</mml:mn></mml:msub></m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>PbTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m from first principles. Physical Review Materials, 2018, 2, .	2.4	16
67	First-principles study of tantalum-arsenic binary compounds. Journal of Applied Physics, 2017, 121, 015101.	2.5	3
68	Using gapped topological surface states of Bi2Se3 films in a field effect transistor. Journal of Applied Physics, 2017, 121, .	2.5	16
69	Tuning the carrier scattering mechanism to effectively improve the thermoelectric properties. Energy and Environmental Science, 2017, 10, 799-807.	30.8	326
70	Pressure-induced insulator-to-metal transitions for enhancing thermoelectric power factor in bismuth telluride-based alloys. Physical Chemistry Chemical Physics, 2017, 19, 12784-12793.	2.8	23
71	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
72	Sn2Se3: A conducting crystalline mixed valent phase change memory compound. Journal of Applied Physics, 2017, 121, .	2.5	9

#	Article	IF	Citations
73	Infrared absorption and visible transparency in heavily doped p-type BaSnO3. Applied Physics Letters, 2017, 110, 051904.	3.3	11
74	Thermoelectric properties of AMg₂X₂, AZn₂Sb₂(A =) Tj ETQq0 0 0 rgBT /Overlock 1 Materials Chemistry A, 2017, 5, 8499-8509.	10.3	83
75	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> Physical Review Applied, 2017, 7, .	3.8	36
76	Bandgap Control via Structural and Chemical Tuning of Transition Metal Perovskite Chalcogenides. Advanced Materials, 2017, 29, 1604733.	21.0	154
77	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
78	Computational modelling of the thermoelectric properties of p-type Zintl compound CaMg2Bi2. Materials Today Physics, 2017, 2, 40-45.	6.0	40
79	Dynamic Optical Tuning of Interlayer Interactions in the Transition Metal Dichalcogenides. Nano Letters, 2017, 17, 7761-7766.	9.1	46
80	Ion exchange-prepared NaSbSe₂ nanocrystals: electronic structure and photovoltaic properties of a new solar absorber material. RSC Advances, 2017, 7, 45470-45477.	3.6	11
81	Properties of the antiferromagnetic selenite MnSeO3 and its non-magnetic analogue ZnSnO3 from first principles calculations. Journal of Physics Condensed Matter, 2017, 29, 405501.	1.8	7
82	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
83	Sn(II)-Containing Phosphates as Optoelectronic Materials. Chemistry of Materials, 2017, 29, 2459-2465.	6.7	17
84	New stable ternary alkaline-earth metal Pb(II) oxides: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ca</mml:mi><mml:mo>/</mml mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaPbO</mml:mi><mml:mn>2</mml:mn></mml:msub></ Physical Review Materials, 2017, 1, .	2.4	10
85	Electronic fitness function for screening semiconductors as thermoelectric materials. Physical Review Materials, 2017, 1, .	2.4	98
86	Properties of the ferroelectric visible light absorbing semiconductors: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sn</mml:mi><mml:mn>2</mml:mn></mml: mathvariant="normal">P</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sn</mml:mi><mml:mn>2</mml:mn></mml:mn></mml:	2.4	23
87	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
88	Modulation of electronic properties from stacking orders and spin-orbit coupling for 3R-type MoS2. Scientific Reports, 2016, 6, 24140.	3.3	23
89	On the tuning of electrical and thermal transport in thermoelectrics: an integrated theoryâ€“experiment perspective. Npj Computational Materials, 2016, 2, .	8.7	399
90	Nonrigid band shift and nonmonotonic electronic structure changes upon doping in the normal state of the pnictide high-temperature superconductor<mml:math		

#	Article	IF	Citations
91	Stability, electronic structures and thermoelectric properties of binary Znâ€“Sb materials. Journal of Materials Chemistry C, 2016, 4, 11305-11312.	5.5	19
92	Optical and electronic properties of semiconducting Sn2S3. Applied Physics Letters, 2016, 109, .	3.3	14
93	Thermoelectric properties of n-type SrTiO3. APL Materials, 2016, 4, .	5.1	71
94	Identification and properties of the non-cubic phases of Mg2Pb. AIP Advances, 2016, 6, 125108.	1.3	3
95	Optic phonons and anisotropic thermal conductivity in hexagonal Ge2Sb2Te5. Scientific Reports, 2016, 6, 37076.	3.3	44
96	Perspective: n-type oxide thermoelectrics via visual search strategies. APL Materials, 2016, 4, .	5.1	42
97	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
98	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
99	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
100	Intrinsic ultralow lattice thermal conductivity of the unfilled skutterudite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>FeSb</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2016, 94, .	3.2	23
101	Adsorption and diffusion of Li with S on pristine and defected graphene. Physical Chemistry Chemical Physics, 2016, 18, 31268-31276.	2.8	9
102	Competing covalent and ionic bonding in Ge-Sb-Te phase change materials. Scientific Reports, 2016, 6, 25981.	3.3	35
103	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
104	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:mrow></mml:math> Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 102 Td (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Z</mml:mi><mml:mi>T</mml:mi></m. Physical Review Applied, 2016, 5, .	3.8	45
105	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
106	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: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:mrow></mml:math>. Physical Review Letters, 2015, 115, .	3.8	84
107	<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:mi mathvariant="normal">F</mml:mi></mml:mrow></mml:math>(<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 102 Td (xml	3.2	36
108	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

#	Article	IF	Citations
109	Transport properties of cubic crystalline Ge2Sb2Te5: A potential low-temperature thermoelectric material. Applied Physics Letters, 2015, 106, .	3.3	17
110	Magnetism in Na-filled Fe-based skutterudites. Scientific Reports, 2015, 5, 10782.	3.3	12
111	Electronic, transport, and optical properties of bulk and mono-layer PdSe2. Applied Physics Letters, 2015, 107, .	3.3	170
112	Transparent conducting properties of SrSnO₃ and ZnSnO₃. APL Materials, 2015, 3, 062505.	5.1	65
113	Structural stability of single-layer MoS₂ under large strain. Journal of Physics Condensed Matter, 2015, 27, 105401.	1.8	29
114	Defect-enhanced void filling and novel filled phases of open-structure skutterudites. Chemical Communications, 2015, 51, 10823-10826.	4.1	11
115	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:math><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:m. Physical Review Applied, 2015, 3, .	3.8	178
116	Tuning optical properties of transparent conducting barium stannate by dimensional reduction. APL Materials, 2015, 3, .	5.1	29
117	Dimensionality Controlled Octahedral Symmetry-Mismatch and Functionalities in Epitaxial LaCoO₃/SrTiO₃ Heterostructures. Nano Letters, 2015, 15, 4677-4684.	9.1	71
118	The Electronic Properties of Single-Layer and Multilayer MoS₂ under High Pressure. Journal of Physical Chemistry C, 2015, 119, 10189-10196.	3.1	89
119	Pressure evolution of the potential barriers for transformations of layered BN to dense structures. RSC Advances, 2015, 5, 87550-87555.	3.6	3
120	Ba2TeO as an optoelectronic material: First-principles study. Journal of Applied Physics, 2015, 117, 195705.	2.5	3
121	Complex doping of group 13 elements In and Ga in caged skutterudite CoSb3. Acta Materialia, 2015, 85, 112-121.	7.9	29
122	2DEGs at Perovskite Interfaces between KTaO3 or KNbO3 and Stannates. PLoS ONE, 2014, 9, e91423.	2.5	32
123	Strain dependence of the optical properties and band gap of transparent conducting BaSnO₃and SrSnO₃. Proceedings of SPIE, 2014, , .	0.8	0
124	Strain effects on the band gap and optical properties of perovskite SrSnO3 and BaSnO3. Applied Physics Letters, 2014, 104, .	3.3	108
125	Heavy element doping for enhancing thermoelectric properties of nanostructured zinc oxide. RSC Advances, 2014, 4, 6363.	3.6	61
126	Light scattering and surface plasmons on small spherical particles. Light: Science and Applications, 2014, 3, e179-e179.	16.6	450

#	Article	IF	Citations
127	High temperature thermoelectric properties of rock-salt structure PbS. Solid State Communications, 2014, 182, 34-37.	1.9	13
128	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
129	Optical properties of cubic and rhombohedral GeTe. Journal of Applied Physics, 2013, 113, .	2.5	21
130	Electronic and thermoelectric properties of CoSbS and FeSbS. Physical Review B, 2013, 87, .	3.2	45
131	High Three-Dimensional Thermoelectric Performance from Low-Dimensional Bands. Physical Review Letters, 2013, 110, 146601.	7.8	131
132	Crystal, magnetic and electronic structures and properties of new BaMnPnF (Pn = As, Sb, Bi). Scientific Reports, 2013, 3, 2154.	3.3	27
133	Importance of non-parabolic band effects in the thermoelectric properties of semiconductors. Scientific Reports, 2013, 3, 3168.	3.3	147
134	Thermoelectric properties of Î²-FeSi2. Journal of Applied Physics, 2013, 114, .	2.5	23
135	Itinerant origin of the ferromagnetic quantum critical point in Fe(Ga,Ge)3. Physical Review B, 2013, 88, .	3.2	25
136	Itinerant magnetism in doped semiconducting Î²-FeSi2 and CrSi2. Scientific Reports, 2013, 3, 3517.	3.3	10
137	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
138	Electronic structure and upper critical field of superconducting Ta<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>PdS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 88, .	3.2	21
139	Potential thermoelectric performance of hole-doped Cu₂O. New Journal of Physics, 2013, 15, 043029.	2.9	47
140	ELECTRONIC AND TRANSPORT PROPERTIES OF THERMOELECTRIC Ru2Si3. Functional Materials Letters, 2013, 06, 1340013.	1.2	3
141	Very heavily electron-doped CrSi₂as a high-performance high-temperature thermoelectric material. New Journal of Physics, 2012, 14, 033045.	2.9	31
142	The solid state as a fabric for intertwining chemical bonding, electronic structure and magnetism. , 2012, , .		0
143	Electronic structure and fermiology of superconducting LaNiGa<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	14
144	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

#	Article	IF	Citations
145	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
146	La-Driven Morphotrophic Phase Boundary in the Bi(Zn_{1/2}Ti_{1/2})O₃â€“La(Zn_{1/2}Ti_{1/2})O₃â€“PbTiO₃ Solid Solution. Chemistry of Materials, 2012, 24, 4477-4482.	7.7	16
147	Thermoelectric properties of n-type PbSe revisited. Journal of Applied Physics, 2012, 111, 123701.	2.5	18
148	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
149	Crystal structure and cation off-centering in Bi(Mg<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 602 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inlin. Physical Review B, 2012, 86, .	3.2	11
150	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
151	Three-dimensional magnetism and coupling to the conduction electrons in PdCrO<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, 85, .	3.2	14
152	Optical properties of PbTe and PbSe. Physical Review B, 2012, 85, .	3.2	72
153	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
154	Antiferromagnetism in a Technetium Oxide. Structure of CaTcO₃. Journal of the American Chemical Society, 2011, 133, 1654-1657.	13.7	38
155	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
156	Structure and Properties of Single Crystalline CaMg₂Bi₂, EuMg₂Bi₂, and YbMg₂Bi₂. Inorganic Chemistry, 2011, 50, 11127-11133.	4.0	74
157	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 Physical Review X, 2011, 1, .	8.9	36
158	Transport and optical properties of heavily hole-doped semiconductors BaCu2Se2 and BaCu2Te2. Journal of Solid State Chemistry, 2011, 184, 2744-2750.	2.9	25
159	Variation of physical properties in the nominal Sr4V2O6Fe2As2. Physica C: Superconductivity and Its Applications, 2011, 471, 143-149.	1.2	18
160	Spin glass and semiconducting behavior in one-dimensional BaFe2â^'Î´Se3(Î´â‰ˆ0.2)crystals. Physical Review B, 2011, 84, .	3.2	58
161	Transport properties of hole-doped CuBiS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow Cooperative behavior of Zn cations in Bi-based perovskites: A comparison of (Bi,Sr)<mml:math. Physical	3.2	19
162	xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>ZnNbO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>6</mml:mn></mml:mro	3.2	6

#	Article	IF	Citations
163	First principles prediction of a morphotropic phase boundary in the Bi(Zn1/2Ti1/2)O3â^'(Bi1/2Sr1/2)(Zn1/2Nb1/2)O3 alloy. Applied Physics Letters, 2011, 98, .	3.3	7
164	Chemistry and electronic structure of iron-based superconductors. MRS Bulletin, 2011, 36, 614-619.	3.5	35
165	Electronic Transport in Old and New Thermoelectric Materials. Science of Advanced Materials, 2011, 3, 561-570.	0.7	16
166	Electronic structure calculations with the Tran-Blaha modified Becke-Johnson density functional. Physical Review B, 2010, 82, .	3.2	292
167	THERMOPOWER OF SnTe FROM BOLTZMANN TRANSPORT CALCULATIONS. Functional Materials Letters, 2010, 03, 223-226.	1.2	50
168	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
169	Doping-dependent thermopower of PbTe from Boltzmann transport calculations. Physical Review B, 2010, 81, .	3.2	259
170	Enhanced Born charge and proximity to ferroelectricity in thallium halides. Physical Review B, 2010, 81, .	3.2	72
171	Properties of alkaline-earth-filled skutterudite antimonides:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

#	Article	IF	Citations
181	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
182	Suppression of spin density wave by isoelectronic substitution in. Journal of Solid State Chemistry, 2009, 182, 2326-2331.	2.9	36
183	Electron-phonon superconductivity in noncentrosymmetricLaNiC2: First-principles calculations. Physical Review B, 2009, 80, .	3.2	34
184	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
185	Influence of band structure on the large thermoelectric performance of lanthanum telluride. Physical Review B, 2009, 79, .	3.2	129
186	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:mrow><mml:mn>2</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:mtext>ZrH</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 80, .	3.2	57
187	Nanostructuring and more. Nature Materials, 2008, 7, 616-617.	27.5	55
188	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></mml:math>. Physical Review Letters, 2008, 101, 117004.	7.6	980
189	Electronic Structure, Magnetism and Spin-Fluctuations in Fe-As Based Superconductors. Materials Research Society Symposia Proceedings, 2008, 1148, 1.	0.1	0
190	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:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>: Electronic structure, phonons, and electron-phonon superconductivity. Physical Review B, 2008, 78, .	3.2	81
191	BoltzTraP. A code for calculating band-structure dependent quantities. Computer Physics Communications, 2006, 175, 67-71.	7.5	4,184
192	Electronic structure and lattice distortions inPbMg1â•3Nb2â•3O3studied with density functional theory using the linearized augmented plane-wave method. Physical Review B, 2006, 73, .	3.2	28
193	Electronic structure and transport in type-I and type-VIII clathrates containing strontium, barium, and europium. Physical Review B, 2003, 68, .	3.2	251
194	Theoretical Considerations for Finding New Thermoelectric Materials. Materials Research Society Symposia Proceedings, 2001, 691, 1.	0.1	2
195	Chapter 5 Theoretical and computational approaches for identifying and optimizing novel thermoelectric materials. Semiconductors and Semimetals, 2001, , 125-177.	0.7	48
196	Possible coexistence of rotational and ferroelectric lattice distortions in rhombohedralPbZrxTi1â˜xO3. Physical Review B, 2001, 63, .	3.2	93
197	Prediction of room-temperature high-thermoelectric performance in n-type La(Ru1â˜xRhx)4Sb12. Applied Physics Letters, 1999, 74, 3666-3668.	3.3	32
198	Theory of angular magnetoresistance oscillations inTl2Ba2CuO6. Physical Review B, 1999, 60, 6312-6315.	3.2	16

#	Article	IF	Citations
199	Electronic structure and thermoelectric prospects of phosphide skutterudites. Physical Review B, 1999, 59, 9722-9724.	3.2	76
200	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
201	Magnetoelectronic effects in pyrochloreTl2Mn2O7: Role of Tl-O covalency. Physical Review B, 1997, 55, 313-316.	3.2	83
202	Ferromagnetic Spin Fluctuation Induced Superconductivity inSr2RuO4. Physical Review Letters, 1997, 79, 733-736.	7.8	311
203	Magnetic and electronic properties ofLiMnO2s. Physical Review B, 1997, 55, 309-312.	3.2	51
204	Density functional studies of PbZrO3, KTaO3and KNbO3. Ferroelectrics, 1997, 194, 299-322.	0.6	28
205	Stability and phonons ofKTaO3. Physical Review B, 1996, 53, 176-180.	3.2	103
206	Electronic structure of Ce-filled skutterudites. Physical Review B, 1996, 53, 1103-1108.	3.2	171
207	Electronic and magnetic properties of the 4d itinerant ferromagnet SrRuO3. Journal of Applied Physics, 1996, 79, 4818.	2.5	176
208	Electronic structure and half-metallic transport in theLa1â^'xCaxMnO3system. Physical Review B, 1996, 53, 1146-1160.	3.2	750
209	Electronic properties of YNi2B2C. Solid State Communications, 1996, 98, 899-902.	1.9	32
210	Electronic structure of heazlewooditeNi3S2. Physical Review B, 1996, 54, 13542-13545.	3.2	21
211	Noncollinear Intra-atomic Magnetism. Physical Review Letters, 1996, 76, 4420-4423.	7.8	170
212	Regularities Among the Classes of High Temperature Superconductors: Questions of Pressure. Kluwer International Series in Engineering and Computer Science, 1996, , 449-463.	0.2	1
213	New class of intermetallic borocarbide superconductors: Electron-phonon coupling and physical parameters. Journal of Superconductivity and Novel Magnetism, 1995, 8, 425-428.	0.5	13
214	Unusual oxygen doping behavior in Hg cuprates and its pressure dependence. Journal of Superconductivity and Novel Magnetism, 1995, 8, 769-771.	0.5	0
215	Superconductivity of boro-nitrides. Nature, 1995, 374, 682-682.	27.8	13
216	Structure and energetics of antiferroelectricPbZrO3. Physical Review B, 1995, 52, 12559-12563.	3.2	105

#	Article	IF	Citations
217	Electronic and structural properties ofLa3Ni2B2N3. Physical Review B, 1995, 51, 8668-8671.	3.2	26
218	Local density and generalized gradient approximation studies of KNbO3 and BaTiO3. Ferroelectrics, 1995, 164, 143-152.	0.6	58
219	Relationship ofSr2RuO4to the superconducting layered cuprates. Physical Review B, 1995, 52, 1358-1361.	3.2	262
220	LuNi2B2C: A novel Ni-based strong-coupling superconductor. Physical Review Letters, 1994, 72, 3702-3705.	7.8	291
221	Electronic structure ofPrBa2Cu3O7. Physical Review B, 1994, 50, 4106-4111.	3.2	26
222	Unconventional Oxygen Doping Behavior inHgBa2Ca2Cu3O8+Î´. Physical Review Letters, 1994, 73, 476-479.	7.8	62
223	LaPt2B2C: A conventional borocarbide superconductor. Physical Review B, 1994, 50, 6486-6488.	3.2	25
224	Pressure-dependent electronic structure and doping in HgBa2Ca2Cu3O8+Î´. Physica C: Superconductivity and Its Applications, 1994, 233, 237-241.	1.2	21
225	Electronic structure studies of doped and undoped Hgî—¸Baî—¸Caî—¸Cuî—¸O. Physica C: Superconductivity and Its Applications, 1994, 235-240, 2113-2114.	1.2	6
226	Skutterudite antimonides: Quasilinear bands and unusual transport. Physical Review B, 1994, 50, 11235-11238.	3.2	272
227	Planewaves, Pseudopotentials and the LAPW Method. , 1994, , .		904
228	Electronic structure of HgBa2CuO4. Physica C: Superconductivity and Its Applications, 1993, 212, 228-232.	1.2	49
229	bcc cobalt: Metastable phase or forced structure?. Journal of Applied Physics, 1993, 73, 6189-6191.	2.5	37
230	Weighted-density-approximation ground-state studies of solids. Physical Review B, 1993, 48, 14099-14103.	3.2	27
231	Electronic structure ofHgBa2Ca2Cu3O8: The role of mercury. Physical Review B, 1993, 48, 3571-3574.	3.2	34
232	Elastic instability of bcc cobalt. Physical Review B, 1993, 47, 8515-8519.	3.2	68
233	Arsenic poisoning of magnetism in bcc cobalt. Journal of Applied Physics, 1992, 71, 3431-3433.	2.5	15
234	General-potential study of the electronic and magnetic structure of FeCo. Physical Review B, 1992, 46, 11145-11148.	3.2	36

#	Article	IF	Citations
235	Electronic characteristics of Tl2Ba2CuO6. Physica C: Superconductivity and Its Applications, 1992, 203, 193-202.	1.2	60