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	Wet-chemistry hydrogen doped TiO2 with switchable defects control for photocatalytic hydrogen evolution. Matter, 2022, 5, 206-218.	5.0	66
2	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
3	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, .	1.1	0
4	Low thermal conductivity and high thermoelectric performance via Cd underbonding in half-Heusler PCdNa. Physical Review B, 2022, 105, .	1.1	15
5	Progress of graphdiyne-based materials for anodes of alkali metal ion batteries. Nano Futures, 2022, 6, 022004.	1.0	4
6	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></ Physical Review B, 2022, 105, .	1.1	5
7	Dirac Fermion Cloning, MoirÃ© Flat Bands, and Magic Lattice Constants in Epitaxial Monolayer Graphene. Advanced Materials, 2022, 34, e2200625.	11.1	9
8	Unraveling the relationships between chemical bonding and thermoelectric properties: n-type ABO₃ perovskites. Journal of Materials Chemistry A, 2022, 10, 11039-11045.	5.2	10
9	Favorable Energy Band Alignment of TiO₂ Anatase/Rutile Heterophase Homojunctions Yields Photocatalytic Hydrogen Evolution with Quantum Efficiency Exceeding 45.6% (Adv. Energy) Tj ETQq1 1 0.784314 rgBT /Overlock	10.2	106
10	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ta</mml:mi><mml:mn>4</mml:mn></ : A possible one-dimensional topological insulator. Physical Review B, 2022, 105, .	1.1	21
11	Selfâ€intercalation Tunable Interlayer Exchange Coupling in a Synthetic van der Waals Antiferromagnet. Advanced Functional Materials, 2022, 32, .	7.8	10
12	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>KCo</mml:mi><mml:mn>2</mml:mn></ : A new portal for the physics of high-purity metals. Physical Review Materials, 2022, 6, .	3.2	1
13	Atomically Dispersed MoO_x on Rhodium Metallene Boosts Electrocatalyzed Alkaline Hydrogen Evolution. Angewandte Chemie - International Edition, 2022, 61, .	7.2	57
14	Violation of the rule of parsimony: Mixed local moment and itinerant Fe magnetism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>3</mml:mn></ Physical Review B, 2022, 106, .	1.1	1
15	Designing Rashba systems for high thermoelectric performance based on the van der Waals heterostructure. Materials Today Physics, 2022, 27, 100788.	2.9	1
16	Origin of giant electric-field-induced strain in faulted alkali niobate films. Nature Communications, 2022, 13, .	5.8	11
17	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
18	First-principles study of electronic and optical properties of ternary compounds AuBX2 (X = S, Se, Te) and AuMTe2 (M = Al, In, Ga). Solid State Sciences, 2021, 111, 106508.	1.5	27

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19	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.	1.9	1
20	Disorder and Itinerant Magnetism in Full Heusler Pd2TiIn. Chinese Physics Letters, 2021, 38, 017102.	1.3	1
21	Storage mechanism of K in hydrogen-substituted graphdiyne as a superior anode. Journal of Materials Chemistry A, 2021, 9, 12320-12330.	5.2	4
22	Improved thermoelectric transport properties of Ge₄Se₃Te through dimensionality reduction. Journal of Materials Chemistry C, 2021, 9, 1804-1813.	2.7	17
23	Binary and Ternary Colloidal Cuâ€Snâ€Te Nanocrystals for Thermoelectric Thin Films. Small, 2021, 17, e2006729.	5.2	8
24	Vacancy ordering induced topological electronic transition in bulk Eu ₂ ZnSb ₂. Science Advances, 2021, 7, .	4.7	21
25	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></mml:msub><mml:msub><mml:mi>As</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2021, 103, .	1.1	4
26	Stable Bimetallene Hydride Boosts Anodic CO Tolerance of Fuel Cells. ACS Energy Letters, 2021, 6, 1912-1919.	8.8	48
27	Deformation and ductile fracture of nanocrystalline gold ultrathin nanoribbon: Width effect. Fatigue and Fracture of Engineering Materials and Structures, 2021, 44, 1850-1861.	1.7	5
28	Ferromagnetism in a Semiconductor with Mobile Carriers via Low-Level Nonmagnetic Doping. Physical Review Applied, 2021, 15, .	1.5	3
29	Room-temperature intrinsic ferromagnetism in epitaxial CrTe2 ultrathin films. Nature Communications, 2021, 12, 2492.	5.8	179
30	Zintl chemistry leading to ultralow thermal conductivity, semiconducting behavior, and high thermoelectric performance of hexagonal KBaBi. Physical Review B, 2021, 103, .	1.1	24
31	Thermoelectrics by Computational Design: Progress and Opportunities. Annual Review of Materials Research, 2021, 51, 565-590.	4.3	23
32	Adsorption of K Ions on Single-Layer GeC for Potential Anode of K Ion Batteries. Nanomaterials, 2021, 11, 1900.	1.9	6
33	Interior Melting of Rapidly Heated Gold Nanoparticles. Journal of Physical Chemistry Letters, 2021, 12, 8170-8177.	2.1	6
34	Identification of a low-energy metastable 1T -type phase for monolayer VSe2. Physical Review B, 2021, 104, .	1.1	2
35	Intrinsic nanostructure induced ultralow thermal conductivity yields enhanced thermoelectric performance in Zintl phase Eu2ZnSb2. Nature Communications, 2021, 12, 5718.	5.8	34
36	Type-II Dirac cones and electron-phonon interaction in monolayer biphenylene from first-principles calculations. Physical Review B, 2021, 104, .	1.1	33

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37	Thermoelectric Properties of Zintl Phase YbMg₂Sb₂. Chemistry of Materials, 2020, 32, 776-784.	3.2	40
38	Recent progress of TMD nanomaterials: phase transitions and applications. Nanoscale, 2020, 12, 1247-1268.	2.8	132
39	Bandgap Tunable Ternary Cd_xSb_{2â€“y}S_{3â^Î´} Nanocrystals for Solar Cell Applications. ACS Omega, 2020, 5, 113-121.	1.6	4
40	Prediction of superconductivity and topological aspects in single-layer Î²â^'Bi2Pd. Physical Review B, 2020, 102, .	1.1	10
41	The Effect of Strain Rate on the Deformation Processes of NC Gold with Small Grain Size. Crystals, 2020, 10, 858.	1.0	3
42	Ultralow Thermal Conductivity in Csâ€“Sbâ€“Se Compounds: Lattice Instability versus Lone-Pair Electrons. Chemistry of Materials, 2020, 32, 8906-8913.	3.2	18
43	Giant piezoelectricity in oxide thin films with nanopillar structure. Science, 2020, 369, 292-297.	6.0	86
44	Copper(I)-Based Flexible Organicâ€“Inorganic Coordination Polymer and Analogues: High-Power Factor Thermoelectrics. ACS Applied Materials & Interfaces, 2020, 12, 53841-53851.	4.0	14
45	Defect-mediated Rashba engineering for optimizing electrical transport in thermoelectric BiTeI. Npj Computational Materials, 2020, 6, .	3.5	24
46	Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, .	1.1	27
47	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, .	1.1	5
48	Pressure-driven significant phonon mode softening and robust superconductivity in layered germanium phosphide. Journal of Materials Chemistry A, 2020, 8, 20054-20061.	5.2	17
49	Second Harmonic Generation Susceptibilities from Symmetry Adapted Wannier Functions. Physical Review Letters, 2020, 125, 187402.	2.9	94
50	Localization in the SCAN meta-generalized gradient approximation functional leading to broken symmetry ground states for graphene and benzene. Physical Chemistry Chemical Physics, 2020, 22, 19585-19591.	1.3	8
51	Superstructures and Superconductivity Linked with Pd Intercalation in Nb₂Pd_xSe₅. Chemistry of Materials, 2020, 32, 8361-8366.	3.2	1
52	Enhanced Thermoelectric Performance in Black Phosphorus Nanotubes by Band Modulation through Tailoring Nanotube Chirality. Small, 2020, 16, e2001820.	5.2	13
53	Thermoelectric properties of monolayer GeAsSe and SnSbTe. Journal of Materials Chemistry C, 2020, 8, 9763-9774.	2.7	22
54	Establishing the carrier scattering phase diagram for ZrNiSn-based half-Heusler thermoelectric materials. Nature Communications, 2020, 11, 3142.	5.8	87

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55	Heating-Rate and Particle-Size Effects on Melting Process of Au Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 7414-7420.	1.5	12
56	Bi_{0.5}Sb_{1.5}Te₃-based films for flexible thermoelectric devices. Journal of Materials Chemistry A, 2020, 8, 4552-4561.	5.2	53
57	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, .	1.1	11
58	Achieving high-performance p-type SmMg₂Bi₂ thermoelectric materials through band engineering and alloying effects. Journal of Materials Chemistry A, 2020, 8, 15760-15766.	5.2	21
59	Quantum critical point and ferromagnetic semiconducting behavior in p -type FeAs2. Physical Review B, 2020, 101, .	1.1	5
60	Characterization of rattling in relation to thermal conductivity: Ordered half-Heusler semiconductors. Physical Review B, 2020, 101, .	1.1	43
61	Hydrogen Stabilized RhPdH 2D Bimetallene Nanosheets for Efficient Alkaline Hydrogen Evolution. Journal of the American Chemical Society, 2020, 142, 3645-3651.	6.6	152
62	Defect Engineering for Realizing p-Type AgBiSe₂ with a Promising Thermoelectric Performance. Chemistry of Materials, 2020, 32, 3528-3536.	3.2	17
63	Nanocrystalline gold with small size: inverse Hallâ€“Petch between mixed regime and super-soft regime. Philosophical Magazine, 2020, 100, 2335-2351.	0.7	21
64	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: 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:m. Physical Review B, 2020, 101, .	1.1	17
65	Understanding the lattice thermal conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m from an ab initio perspective. Physical Review Materials, 2020, 4, .	0.9	18
66	Prediction of ternary alkaline-earth metal Sn(II) and Pb(II) chalcogenide semiconductors. Physical Review Materials, 2020, 4, .	0.9	1
67	The thermal and thermoelectric transport properties of SiSb, GeSb and SnSb monolayers. Journal of Materials Chemistry C, 2019, 7, 10652-10662.	2.7	36
68	Electronic structure as a guide in screening for potential thermoelectrics: Demonstration for half-Heusler compounds. Physical Review B, 2019, 100, .	1.1	34
69	Density functional methods for the magnetism of transition metals: SCAN in relation to other functionals. Physical Review B, 2019, 100, .	1.1	42
70	n-Type TaCoSn-Based Half-Heuslers as Promising Thermoelectric Materials. ACS Applied Materials & Interfaces, 2019, 11, 41321-41329.	4.0	44
71	Orthorhombic to monoclinic phase transition in NbNiTe2. Physical Review B, 2019, 100, .	1.1	1
72	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.	5.6	33

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73	Interplay of electronic, magnetic, and structural properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>GdB</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:math> from first principles. Physical Review B, 2019, 100, .	1.1	9
74	Bottom-up growth of homogeneous MoirÃ© superlattices in bismuth oxychloride spiral nanosheets. Nature Communications, 2019, 10, 4472.	5.8	59
75	Understanding the asymmetrical thermoelectric performance for discovering promising thermoelectric materials. Science Advances, 2019, 5, eaav5813.	4.7	52
76	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>3</mml:mn></mml:msub></mml:math> Physical Review B, 2019, 99, .	1.1	11
77	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, .	1.1	0
78	Complex Band Structures and Lattice Dynamics of Bi₂Te₃â€Based Compounds and Solid Solutions. Advanced Functional Materials, 2019, 29, 1900677.	7.8	135
79	High-Throughput Screening for Advanced Thermoelectric Materials: Diamond-Like ABX₂ Compounds. ACS Applied Materials & Interfaces, 2019, 11, 24859-24866.	4.0	72
80	Divalent doping-induced thermoelectric power factor increase in p-type Bi2Te3 via electronic structure tuning. Journal of Applied Physics, 2019, 125, .	1.1	11
81	Achieving band convergence by tuning the bonding ionicity in nâ€type Mg₃Sb₂. Journal of Computational Chemistry, 2019, 40, 1693-1700.	1.5	68
82	Switchable Outâ€ofâ€Plane Polarization in 2D LiAlTe₂. Advanced Electronic Materials, 2019, 5, 1900089.	2.6	20
83	Layered Tl₂O: a model thermoelectric material. Journal of Materials Chemistry C, 2019, 7, 5094-5103.	2.7	46
84	Thermal conductivity of MoS2 monolayers from molecular dynamics simulations. AIP Advances, 2019, 9, .	0.6	22
85	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
86	Multi Band Gap Electronic Structure in CH3NH3PbI3. Scientific Reports, 2019, 9, 2144.	1.6	26
87	Tunable Optical Properties in Sn_xSb_{2â€“y}S₃: A New Solar Absorber Material with an Efficiency of near 5%. Journal of Physical Chemistry C, 2019, 123, 5209-5215.	1.5	12
88	Ba₃CrN₃H: A New Nitride-Hydride with Trigonal Planar Cr⁴⁺. Inorganic Chemistry, 2019, 58, 3302-3307.	1.9	16
89	Molecular Bridge Thermal Diode Enabled by Vibrational Mismatch. Physical Review Applied, 2019, 11, .	1.5	11
90	Storage of Na in layered graphdiyne as high capacity anode materials for sodium ion batteries. Journal of Materials Chemistry A, 2019, 7, 25609-25618.	5.2	20

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91	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></m through hydrogen doping. Physical Review B, 2019, 100, .	1.3	15
92	Melting of Nanocrystalline Gold. Journal of Physical Chemistry C, 2019, 123, 907-914.	1.5	4
93	Discovery of TaFeSb-based half-Heuslers with high thermoelectric performance. Nature Communications, 2019, 10, 270.	5.8	227
94	Adsorption of Na on silicene for potential anode for Na-ion batteries. Electrochimica Acta, 2019, 297, 497-503.	2.6	35
95	First principles based screen for identification of transparent conductors. Journal of Materials Chemistry C, 2019, 7, 2436-2442.	2.7	5
96	Adsorption of Li on single-layer silicene for anodes of Li-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 8887-8896.	1.3	62
97	Thermoelectric properties of layered NaSbSe₂. Journal of Physics Condensed Matter, 2018, 30, 225501.	0.7	10
98	Synthesis and Crystal Structure of the Layered Lanthanide Oxychlorides Ba₃Ln₂O₅Cl₂. Inorganic Chemistry, 2018, 57, 1727-1734.	1.9	9
99	Reemergence of high-Tc superconductivity in the (Li1-xFe x)OHFe1-ySe under high pressure. Nature Communications, 2018, 9, 380.	5.8	60
100	Orbital controlled band gap engineering of tetragonal BiFeO₃ for optoelectronic applications. Journal of Materials Chemistry C, 2018, 6, 1239-1247.	2.7	80
101	Collective-Goldstone-mode-induced ultralow lattice thermal conductivity in Sn-filled skutterudite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SnFe</mml:mi><mml:mn>4</mml:mn></ Physical Review B, 2018, 97, .	1.1	11
102	Large thermoelectric power factor from crystal symmetry-protected non-bonding orbital in half-Heuslers. Nature Communications, 2018, 9, 1721.	5.8	111
103	Bismuth and antimony-based oxyhalides and chalcohalides as potential optoelectronic materials. Npj Computational Materials, 2018, 4, .	3.5	86
104	Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures. MRS Advances, 2018, 3, 397-402.	0.5	5
105	<scp>Pb₅Sb₈S₁₇</scp> quantum dotâ€sensitized solar cells with an efficiency of 6% under 0.05 sun: <scp>T</scp>heoretical and experimental studies. Progress in Photovoltaics: Research and Applications, 2018, 26, 205-213.	4.4	13
106	First principles study on 2Hâ€“1Tâ€² transition in MoS₂ with copper. Physical Chemistry Chemical Physics, 2018, 20, 26986-26994.	1.3	39
107	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
108	Applicability of the Strongly Constrained and Appropriately Normed Density Functional to Transition-Metal Magnetism. Physical Review Letters, 2018, 121, 207201.	2.9	118

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109	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	3.5	107
110	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
111	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, 187002.	2.9	16
112	Modulation of Hydrogen Evolution Catalytic Activity of Basal Plane in Monolayer Platinum and Palladium Dichalcogenides. ACS Omega, 2018, 3, 10058-10065.	1.6	46
113	Thermoelectric properties of p-type cubic and rhombohedral GeTe. Journal of Applied Physics, 2018, 123, .	1.1	40
114	Optimal Bandgap in a 2D Ruddlesdenâ€“Popper Perovskite Chalcogenide for Single-Junction Solar Cells. Chemistry of Materials, 2018, 30, 4882-4886.	3.2	49
115	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
116	Tunability of electronic and optical properties of the Baâ€“Zrâ€“S system via dimensional reduction. European Physical Journal B, 2018, 91, 1.	0.6	16
117	Giant optical anisotropy in a quasi-one-dimensional crystal. Nature Photonics, 2018, 12, 392-396.	15.6	269
118	Spin-orbit coupled systems in the atomic limit: rhenates, osmates, iridates. Physical Review B, 2018, 97, .	1.1	25
119	Discovery of ZrCoBi based half Heuslers with high thermoelectric conversion efficiency. Nature Communications, 2018, 9, 2497.	5.8	243
120	Optical and electronic properties of doped p -type CuI: Explanation of transparent conductivity from first principles. Physical Review Materials, 2018, 2, .	0.9	7
121	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, .	0.9	16
122	First-principles study of tantalum-arsenic binary compounds. Journal of Applied Physics, 2017, 121, 015101.	1.1	3
123	Using gapped topological surface states of Bi2Se3 films in a field effect transistor. Journal of Applied Physics, 2017, 121, .	1.1	16
124	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
125	Tuning the carrier scattering mechanism to effectively improve the thermoelectric properties. Energy and Environmental Science, 2017, 10, 799-807.	15.6	326
126	Pressure-induced insulator-to-metal transitions for enhancing thermoelectric power factor in bismuth telluride-based alloys. Physical Chemistry Chemical Physics, 2017, 19, 12784-12793.	1.3	23

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127	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.	4.0	42
128	Sn2Se3: A conducting crystalline mixed valent phase change memory compound. Journal of Applied Physics, 2017, 121, .	1.1	9
129	Interacting nanoscale magnetic superatom cluster arrays in molybdenum oxide bronzes. Nanoscale, 2017, 9, 7922-7929.	2.8	6
130	Infrared absorption and visible transparency in heavily doped p-type BaSnO3. Applied Physics Letters, 2017, 110, 051904.	1.5	11
131	Thermoelectric properties of AMg₂X₂, AZn₂Sb₂(A =) Tj ETQq1 1 0.784314 rgBT O Materials Chemistry A, 2017, 5, 8499-8509.	5.2	83
132	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><mml: Physical Review Applied, 2017, 7, .	1.5	36
133	Bandgap Control via Structural and Chemical Tuning of Transition Metal Perovskite Chalcogenides. Advanced Materials, 2017, 29, 1604733.	11.1	154
134	Thermal conductivity of single-layer WSe₂ by a Stillingerâ€“Weber potential. Nanotechnology, 2017, 28, 075708.	1.3	33
135	Non-Fermi surface nesting driven commensurate magnetic ordering in Fe-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">S</mml:mi><mml:msub><mml:mi mathvariant="normal">r</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>Ru</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2017, 95, .	1.1	4
136	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
137	The curious case of cuprous chloride: Giant thermal resistance and anharmonic quasiparticle spectra driven by dispersion nesting. Physical Review B, 2017, 96, .	1.1	23
138	Computational modelling of the thermoelectric properties of p-type Zintl compound CaMg2Bi2. Materials Today Physics, 2017, 2, 40-45.	2.9	40
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289	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
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