Yuan-xu Wang

List of Publications by Year
in descending order

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		109137	155451
170	4,316	35	55
papers	citations	h-index	g-index

172	172	172	4832
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	C3N monolayers as promising candidates for NO2 sensors. Sensors and Actuators B: Chemical, 2018, 266, 664-673.	4.0	172
2	Enhanced visible-light photocatalytic activity of a g-C₃N₄/BiVO₄nanocomposite: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 10218-10226.	1.3	157
3	The new understanding on photocatalytic mechanism of visible-light response NS codoped anatase TiO2 by first-principles. Applied Catalysis B: Environmental, 2013, 142-143, 45-53.	10.8	151
4	Enhanced photocatalytic H2-production activity of bicomponent NiO/TiO2 composite nanofibers. Journal of Colloid and Interface Science, 2015, 449, 115-121.	5.0	136
5	Lithium Doping to Enhance Thermoelectric Performance of MgAgSb with Weak Electronâ€“Phonon Coupling. Advanced Energy Materials, 2016, 6, 1502269.	10.2	122
6	Elastic and electronic properties of TcB2 and superhard ReB2: First-principles calculations. Applied Physics Letters, 2007, 91, .	1.5	118
7	Enhanced photocatalytic oxidation of propylene over V-doped TiO2 photocatalyst: Reaction mechanism between V5+ and single-electron-trapped oxygen vacancy. Applied Catalysis B: Environmental, 2015, 176-177, 160-172.	10.8	78
8	Giant Piezoelectric Effects in Monolayer Group-V Binary Compounds with Honeycomb Phases: A First-Principles Prediction. Journal of Physical Chemistry C, 2017, 121, 25576-25584.	1.5	78
9	Valence mediated tunable magnetism and electronic properties by ferroelectric polarization switching in 2D FeI₂/In₂Se₃ van der Waals heterostructures. Nanoscale, 2019, 11, 9931-9936.	2.8	75
10	Ab initio simulation studies on the room-temperature ferroelectricity in two-dimensional Î² -phase GeS. Applied Physics Letters, 2019, 114, .	1.5	72
11	High thermoelectric performance in Cu₂Se superionic conductor with enhanced liquid-like behaviour by dispersing SiC. Journal of Materials Chemistry A, 2019, 7, 7006-7014.	5.2	71
12	Outstanding thermoelectric performances for both p- and n-type SnSe from first-principles study. Journal of Alloys and Compounds, 2015, 644, 615-620.	2.8	65
13	No quenching of magnetic moment for the GenCoâ€ˆ(n=1â€“13) clusters: First-principles calculations. Journal of Chemical Physics, 2008, 128, 124319.	1.2	62
14	Geometries, stabilities, and electronic properties of (n=9â€“16) clusters: Density-functional theory investigations. Chemical Physics, 2008, 352, 291-296.	0.9	60
15	Phase Stability and Physical Properties of Manganese Borides: A First-Principles Study. Journal of Physical Chemistry C, 2011, 115, 21429-21435.	1.5	60
16	First-principles study of the electronic structure and optical properties of Ce-doped ZnO. Journal of Applied Physics, 2011, 109, .	1.1	55
17	Dual effects of lone-pair electrons and rattling atoms in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CuBiS</mml:mi><mml:mn>2</mml:mn></mml:msub><in on its ultralow thermal conductivity. Physical Review B, 2017, 96, .	1.1	52
18	Marcasite osmium nitride with high bulk modulus: First-principles calculations. Applied Physics Letters, 2007, 90, 061922.	1.5	50

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19	Ab initiostudy of monoclinic iridium nitride as a high bulk modulus compound. Physical Review B, 2007, 75, .	1.1	50
20	Possible Origin of Ferromagnetism in an Undoped ZnO d0 Semiconductor. Journal of Physical Chemistry C, 2012, 116, 9709-9715.	1.5	50
21	The structural and electronic properties of Li-doped fluorinated graphene and its application to hydrogen storage. International Journal of Hydrogen Energy, 2012, 37, 5754-5761.	3.8	50
22	Hybrid density functional study on the mechanism for the enhanced photocatalytic properties of the ultrathin hybrid layered nanocomposite g-C3N4/BiOCl. Applied Surface Science, 2018, 435, 1351-1360.	3.1	50
23	Geometries, stabilities, and magnetic properties of MnGe (n= 2â€“16) clusters: Density-functional theory investigations. Computational and Theoretical Chemistry, 2009, 901, 18-23.	1.5	49
24	First-principles study of the (001) surface of cubicCaTiO3. Physical Review B, 2006, 73, .	1.1	48
25	Structural, mechanical, and electronic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0104.gif" overflow="scroll"><mml:msub><mml:mrow><mml:mi>TaB</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow TaB, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0105.gif" overflow="scroll"><mml:msub><mml:mrow><mml:mi>IrB</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> and IrB: First-principle calculation. Journal of Solid State Chemistry, 2009, 182, 2880-2886.	1.4	47
26	Density-functional study of structural, electronic, and magnetic properties of the EuSinâ€ˆ(n=1â€“13) clusters. Journal of Chemical Physics, 2009, 131, 114312.	1.2	46
27	Effects of Mo/W codoping on the visible-light photocatalytic activity of monoclinic BiVO₄ within the GGA + U framework. RSC Advances, 2016, 6, 12290-12297.	1.7	44
28	Coreâ€“shell nanostructures introduce multiple potential barriers to enhance energy filtering for the improvement of the thermoelectric properties of SnTe. Nanoscale, 2020, 12, 1904-1911.	2.8	43
29	Structural and electronic properties of ZnO under high pressure. Journal of Alloys and Compounds, 2009, 476, 306-310.	2.8	42
30	Low effective mass leading to an improved ZT value by 32% for n-type BiCuSeO: a first-principles study. Journal of Materials Chemistry A, 2014, 2, 13923.	5.2	42
31	Thermoelectric properties of monolayer Sb2Te3. Journal of Applied Physics, 2018, 124, .	1.1	42
32	Î³-GeSe: A two-dimensional ferroelectric material with doping-induced ferromagnetism. Applied Physics Letters, 2019, 115, .	1.5	41
33	Investigation of tetragonal ReN2 and WN2 with high shear moduli from first-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 2569-2574.	0.9	39
34	InTeI: a novel wide-bandgap 2D material with desirable stability and highly anisotropic carrier mobility. Nanoscale, 2020, 12, 5888-5897.	2.8	39
35	Crystal structure, electronic structure, and thermoelectric properties of Ca5Al2Sb6. Journal of Materials Chemistry, 2011, 21, 12497.	6.7	38
36	Enhanced photocatalytic activities of Bi₂WO₆ by introducing Zn to replace Bi lattice sites: a first-principles study. RSC Advances, 2015, 5, 29058-29065.	1.7	38

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37	New monolayer ternary In-containing sesquichalcogenides BiInSe₃, SbInSe₃, BiInTe₃, and SbInTe₃ with high stability and extraordinary piezoelectric properties. Physical Chemistry Chemical Physics, 2018, 20, 19177-19187.	1.3	38
38	Thermoelectric optimization of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>AgBiS</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> by defect engineering for room-temperature applications. Physical Review B, 2019, 99, .	1.1	38
39	The competition of double-, four-, and three-ring tubular B3nâ€^(n=8â€“32) nanoclusters. Journal of Chemical Physics, 2008, 129, 024903.	1.2	36
40	Structure, stability, and magnetism of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Sc</mml:mi><mml:mi>n</mml:mi></mml:msub><mml:mi mathvariant="normal">Al</mml:mi></mml:mrow></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>(</mml:mo><mml:mi>n</mml:mi><mml:mo>=</mml:mo><mml:mn>1</mml:mn><mml:mo>â€	1.0	35
41	A new hard phase of ReB4 predicted from first principles. Journal of Alloys and Compounds, 2013, 573, 20-26.	2.8	34
42	Boron-decorated C₉N₄ monolayers as promising metal-free catalysts for electrocatalytic nitrogen reduction reaction: a first-principles study. New Journal of Chemistry, 2020, 44, 422-427.	1.4	34
43	Predicted boron-carbide compounds: A first-principles study. Journal of Chemical Physics, 2014, 140, 224704.	1.2	33
44	Structural, electronic and magnetic properties of GdSi (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 477 Td (xmlns:mml="http://ww clusters: A density functional study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 1120-1127.	0.9	32
45	Transition metal embedded C₃N monolayers as promising catalysts for the hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2019, 21, 20432-20441.	1.3	32
46	Enhancement of Thermoelectric Properties in Pdâ€“In Co-Doped SnTe and Its Phase Transition Behavior. ACS Applied Materials & Interfaces, 2019, 11, 33792-33802.	4.0	32
47	First-Principles Study of the (001) Surface of Cubic SrHfO3 and SrTiO3. Journal of Physical Chemistry B, 2005, 109, 12909-12913.	1.2	31
48	Enhancement of thermoelectric figure of merit by the insertion of multi-walled carbon nanotubes in Î±-MgAgSb. Applied Physics Letters, 2018, 113, .	1.5	31
49	Endowing single-electron-trapped oxygen vacancy self-modified titanium dioxide with visible-light photocatalytic activity by grafting Fe(III) nanocluster. Applied Catalysis B: Environmental, 2015, 172-173, 37-45.	10.8	30
50	Ag-Mg antisite defect induced high thermoelectric performance of Î±-MgAgSb. Scientific Reports, 2017, 7, 2572.	1.6	28
51	A theoretical study on structural and electronic properties of Zr-doped B clusters: ZrBn (n=1â€“12). Chemical Physics, 2008, 351, 1-6.	0.9	27
52	First principles studies of phase stability, electronic and elastic properties in BBi compound. Computational Materials Science, 2010, 47, 968-972.	1.4	27
53	The high thermopower of the Zintl compound Sr₅Sn₂As₆ over a wide temperature range: first-principles calculations. Journal of Materials Chemistry A, 2014, 2, 15159-15167.	5.2	27
54	Improved thermoelectric performance of CuGaTe2 with convergence of band valleys: a first-principles study. RSC Advances, 2014, 4, 28714.	1.7	27

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55	Theoretical investigation of the effects of doping on the electronic structure and thermoelectric properties of ZnO nanowires. Physical Chemistry Chemical Physics, 2014, 16, 3771.	1.3	27
56	A graphene-coupled Bi₂WO₆ nanocomposite with enhanced photocatalytic performance: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 14113-14121.	1.3	27
57	Enhanced piezoelectricity of monolayer phosphorene oxides: a theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 27508-27515.	1.3	27
58	A density functional study of YnAl (n=1â€“14) clusters. Journal of Chemical Physics, 2007, 127, 234312.	1.2	26
59	Ultraâ€incompressible and hard technetium carbide and rhenium carbide: Firstâ€principles prediction. Physica Status Solidi - Rapid Research Letters, 2008, 2, 126-128.	1.2	26
60	Investigation of osmium carbides with various stoichiometries: First-principles calculations. Journal of Applied Physics, 2010, 107, .	1.1	26
61	Firstâ€principles study of CrB₄ as a high shear modulus compound. Physica Status Solidi - Rapid Research Letters, 2011, 5, 13-15.	1.2	25
62	First-principles study of the elastic properties of and alloys. Solid State Communications, 2011, 151, 238-241.	0.9	25
63	High Thermoelectric Performance of SnTe by the Synergistic Effect of Alloy Nanoparticles with Elemental Elements. ACS Applied Energy Materials, 2019, 2, 7354-7363.	2.5	25
64	First-principles study of zinc-blende to rocksalt phase transition in BP and BAs. Computational Materials Science, 2009, 44, 1386-1389.	1.4	24
65	Electronic structure and thermoelectric performance of Zintl compound Ca5Ga2As6. Journal of Materials Chemistry, 2012, 22, 20284.	6.7	24
66	Structural phase transitions in MgH2 under high pressure. Solid State Communications, 2008, 148, 403-405.	0.9	23
67	Phase Stability and Elastic Properties of Chromium Borides with Various Stoichiometries. ChemPhysChem, 2013, 14, 1245-1255.	1.0	23
68	Calculations show improved photoelectrochemical performance for N, Ce, and Ceâ€‰+â€‰N doped anatase TiO2. Journal of Applied Physics, 2011, 110, 033519.	1.1	22
69	Isoelectronic indium doping for thermoelectric enhancements in BiCuSeO. Applied Surface Science, 2019, 473, 985-991.	3.1	22
70	High-pressure structural, electronic and optical properties of KMgF3: A first-principles study. Journal of Alloys and Compounds, 2009, 484, 597-600.	2.8	21
71	The relationship between the electronic structure and thermoelectric properties of Zintl compounds M2Zn5As4 (M = K, Rb). Physical Chemistry Chemical Physics, 2014, 16, 5661.	1.3	21
72	First-principles investigation on tunable electronic properties and magnetism by polarization in PbTiO₃/BiFeO₃ 2D ferroelectric heterostructures. Journal of Materials Chemistry C, 2019, 7, 463-473.	2.7	21

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73	Mg₂Sn: a potential mid-temperature thermoelectric material. RSC Advances, 2016, 6, 48728-48736.	1.7	20
74	Origin of high thermoelectric performance of FeNb1â^'xZr/HfxSb1â^'ySny alloys: A first-principles study. Scientific Reports, 2016, 6, 33120.	1.6	20
75	First-principles study of W, WN, WN₂, and WN₃. Physica Status Solidi (B): Basic Research, 2010, 247, 54-58.	0.7	19
76	New Crystal Structures of IrB and IrB₂: First-Principles Calculations. Journal of Physical Chemistry C, 2012, 116, 21961-21966.	1.5	19
77	Electronic Structure and Thermoelectric Properties of ZnO Single-Walled Nanotubes and Nanowires. Journal of Physical Chemistry C, 2013, 117, 21037-21042.	1.5	19
78	Tuning magnetism by biaxial strain in native ZnO. Physical Chemistry Chemical Physics, 2015, 17, 16536-16544.	1.3	19
79	Structural stabilities, electronic and optical properties of CaF2 under high pressure: A first-principles study. Computational Materials Science, 2009, 47, 41-45.	1.4	18
80	Giant Magnetoelectric Coupling and Two-Dimensional Electron Gas Regulated by Polarization in BiFeO₃/LaFeO₃ Heterostructures. Journal of Physical Chemistry C, 2019, 123, 16393-16399.	1.5	18
81	Firstâ€principles study of phase transition of tin and lead under high pressure. Physica Status Solidi (B): Basic Research, 2008, 245, 53-57.	0.7	17
82	Nitrogen Vacancies and Oxygen Substitution of Ta₃N₅: First-Principles Investigation. Journal of the Physical Society of Japan, 2014, 83, 114707.	0.7	17
83	The Relation between the Electronic Structure and Thermoelectric Properties for Zintl Compounds Mg₃Sb₂. Journal of the Physical Society of Japan, 2017, 86, 024601.	0.7	17
84	Multifield Control of Domains in a Room-Temperature Multiferroic 0.85BiTi_{0.1}Fe_{0.8}Mg_{0.1}O₃â€“0.15CaTiO₃ Thin Film. ACS Applied Materials & Interfaces, 2018, 10, 20712-20719.	4.0	17
85	Ab initio study of Os_{0.5}W_{0.5}B₂, Re_{0.5}W_{0.5}B₂, and Os_{0.5}Re_{0.5}B₂ with high shear modulus. Physica Status Solidi - Rapid Research Letters, 2009, 3, 106-108.	1.2	16
86	The ground-state structure and physical properties of ReB₃ and IrB₃ predicted from first principles. RSC Advances, 2015, 5, 25919-25928.	1.7	16
87	Origin of different thermoelectric properties between Zintl compounds Ba3Al3P5 and Ba3Ga3P5: A first-principles study. Journal of Alloys and Compounds, 2015, 636, 387-394.	2.8	16
88	Hf/Sb co-doping induced a high thermoelectric performance of ZrNiSn: First-principles calculation. Scientific Reports, 2017, 7, 14590.	1.6	16
89	Tuning the magnetism of two-dimensional hematene by ferroelectric polarization. Physical Chemistry Chemical Physics, 2019, 21, 12301-12309.	1.3	16
90	Predicted crystal structures of molybdenum under high pressure. Journal of Alloys and Compounds, 2013, 556, 116-120.	2.8	15

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91	Engineering electrical transport in Î±-MgAgSb to realize high performances near room temperature. Physical Chemistry Chemical Physics, 2018, 20, 16729-16735.	1.3	15
92	High Thermoelectric Performance of Bi_{0.46}Sb_{1.54}Te₃-SnTe: Synergistic Modulation of Electrical and Thermal Transport by the Introduction of Thermoelectric Hetero Nano Region. ACS Applied Materials & Interfaces, 2019, 11, 36658-36665.	4.0	15
93	First-principles study on the structure instability and electronic structure of cubic Ba0.5Sr0.5TiO3. Solid State Communications, 2005, 135, 290-293.	0.9	14
94	Structural transition of Li3N under high pressure: A first-principles study. Solid State Communications, 2009, 149, 612-615.	0.9	14
95	Pressure-induced phase transition of tantalum mononitride. Thin Solid Films, 2011, 519, 3954-3958.	0.8	14
96	Structural, Electronic, and Thermoelectric Properties of InSe Nanotubes: First-Principles Calculations. Journal of Physical Chemistry C, 2012, 116, 3956-3961.	1.5	14
97	Electronic structure and thermoelectric properties of Zintl compounds A₃AlSb₃ (A = Ca and Sr): first-principles study. RSC Advances, 2015, 5, 65133-65138.	1.7	14
98	Giant magnetic moment of the coreâ€shell Co₁₃@Mn₂₀ clusters: Firstâ€principles calculations. Journal of Computational Chemistry, 2011, 32, 2474-2478.	1.5	13
99	Boron nitride substrate-induced reversible hydrogen storage in bilayer solid matrix via interlayer spacing. International Journal of Hydrogen Energy, 2012, 37, 9677-9687.	3.8	13
100	Pressure induced structural phase transition of OsB2: First-principles calculations. Journal of Solid State Chemistry, 2010, 183, 915-919.	1.4	12
101	Vacancy and Oxygen Substitution for Nitrogen-Induced Structural Stability of Ta₂N₃. Journal of Physical Chemistry C, 2011, 115, 3129-3135.	1.5	12
102	Optical and electrical properties of textured sulfur-hyperdoped silicon: a thermal annealing study. Journal of Materials Science, 2015, 50, 3391-3398.	1.7	12
103	Magneto-Seebeck effect in Co₂FeAl/MgO/Co₂FeAl: first-principles calculations. Physical Chemistry Chemical Physics, 2019, 21, 5803-5812.	1.3	12
104	Predicting excellent anisotropic thermoelectric performance of the layered oxychalcogenides BiAgOCh (Châ€¯=â€¯S, Se, and Te). Computational Materials Science, 2020, 171, 109273.	1.4	12
105	The effect of structure and phase transformation on the mechanical properties of Re₂N and the stability of Mn₂N. Journal of Computational Chemistry, 2012, 33, 18-24.	1.5	11
106	Electronic structure and thermoelectric performance of Zintl compound Sr3GaSb3: A first-principles study. Applied Physics Letters, 2014, 104, .	1.5	11
107	Magnetic domain-wall induced ferroelectric polarization in rare-earth orthoferrites AFeO₃ (A = Lu, Y, Gd): first-principles calculations. Journal of Materials Chemistry C, 2019, 7, 10059-10065.	2.7	11
108	Large anisotropy of electrical conductivity induced high thermoelectric performance of p-type CrSi2. Journal of Alloys and Compounds, 2013, 581, 413-417.	2.8	10

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109	Electronic structure and thermoelectric properties of the Zintl compounds Sr₅Al₂Sb₆ and Ca₅Al₂Sb₆: first-principles study. RSC Advances, 2015, 5, 50720-50728.	1.7	10
110	An impurity intermediate band due to Pb doping induced promising thermoelectric performance of Ca₅In₂Sb₆. Physical Chemistry Chemical Physics, 2015, 17, 15156-15164.	1.3	10
111	Optimizing the Dopant and Carrier Concentration of Ca5Al2Sb6 for High Thermoelectric Efficiency. Scientific Reports, 2016, 6, 29550.	1.6	10
112	Tunable Magnetic Anisotropy and Dzyaloshinskii-Moriya Interaction in an Ultrathin van der Waals Fe3GeTe2/In2Se3 Heterostructure. Frontiers in Physics, 2020, 8, .	1.0	10
113	Excellent thermoelectric performance of BaMgSi driven by low lattice thermal conductivity: A promising thermoelectric material. Journal of Alloys and Compounds, 2020, 827, 154342.	2.8	10
114	Robust manipulation of magnetism in LaAO₃/BaTiO₃ (A = Fe, Mn) Tj ETQq0 0 0 rgBT /Overlock	1.0	10
115	A hard semiconductor OsN₄ with high elastic constant c₄₄. Physica Status Solidi - Rapid Research Letters, 2009, 3, 272-274.	1.2	9
116	Structural, Mechanical Stability, and Physical Properties of Iridium Carbides with Various Stoichiometries: First-Principles Investigations. Journal of Physical Chemistry C, 2011, 115, 6948-6953.	1.5	9
117	Thermoelectric properties of Heusler-type compound Fe2V1â^'xNbxAl. Journal of Applied Physics, 2011, 110, 013530.	1.1	9
118	Pressure effect on the electronic structure and thermoelectric properties of Î±-MgAgSb. Computational Materials Science, 2018, 155, 450-456.	1.4	9
119	Improvement of Thermoelectricity Through Magnetic Interactions in Layered Cr₂Ge₂Te₆. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1800172.	1.2	9
120	Electronic structure and thermoelectric properties of In32â^'xGexO48 (x=0, 1, 2, and 3) at low temperature. Applied Physics Letters, 2010, 97, 252106.	1.5	8
121	Density Functional Study of CO Adsorbed on Mn_N (N = 2â^'8) Clusters. Journal of Physical Chemistry A, 2010, 114, 1616-1620.	1.1	8
122	Impact of Electron Acceptor on Three-Photon Absorption Cross-Section of the Fluorene Derivatives. Journal of Physical Chemistry A, 2012, 116, 7445-7451.	1.1	8
123	First-Principles Study of The Electronic Structure and Thermoelectric Properties of IrN₂. Journal of the Physical Society of Japan, 2013, 82, 104706.	0.7	8
124	A key factor improving the thermoelectric properties of Zintl compounds A5M2Pn6 (A=Ca, Sr, Ba;) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	1.4	8
125	Influence of the elements (Pn = As, Sb, Bi) on the transport properties of p-type Zintl compounds Ba2ZnPn2. Computational Materials Science, 2017, 127, 8-14.	1.4	8
126	Optimum electronic structures for high thermoelectric figure of merit within several isotropic elastic scattering models. Scientific Reports, 2017, 7, 10104.	1.6	8

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127	Electric field induced two-dimensional electron gas and magnetism in LaFeO3/SrTiO3 (0â€¯0â€¯1) heterostructures. Applied Surface Science, 2019, 471, 185-195.	3.1	8
128	Stabilization of Skyrmions in a Nanodisk Without an External Magnetic Field. Physical Review Applied, 2020, 13, .	1.5	8
129	Geometries, Stabilities and Electronic Properties of Au₁₂M (M=Na, Mg, Al, Si, P, S,) Tj ETQq1 1 0.784314 rgBT /O	2.2	8
130	Pressure-induced structural transition in PuTe. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 1693-1696.	0.9	7
131	Seeking large Seebeck effects in LaX(X = Mn and Co)O₃/SrTiO₃ superlattices by exploiting high spin-polarized effects. Physical Chemistry Chemical Physics, 2019, 21, 14973-14983.	1.3	7
132	Ferroelectrically tunable magnetism in BiFeO3/BaTiO3 heterostructure revealed by the first-principles calculations. Journal of Advanced Research, 2020, 24, 371-377.	4.4	7
133	Electronic and optical properties of pure and Ce3+-doped MgS single crystals: A first-principles prediction. Journal of Applied Physics, 2009, 105, 063532.	1.1	6
134	The electronic and magnetic properties of MnScN(Nâ€‰=â€‰2â€“10) clusters. Molecular Physics, 2011, 109, 1957-1965.	0.8	6
135	Electronic structure and thermoelectric properties of In4Se3â^'x (x=0, 0.25, 0.5, 0.75): First-principles calculations. Journal of Alloys and Compounds, 2014, 589, 125-131.	2.8	6
136	Electronic structure and thermoelectric properties of orthorhombic SrLiAs. Journal of Applied Physics, 2014, 116, 033705.	1.1	6
137	A class of rare antiferromagnetic metallic oxides: double perovskite AMn₃V₄O₁₂ (A = Na⁺, Ca²⁺, and) Tj ETQq1 1 0.784314 rgBT /Over 12717-12721.	1.3	6
138	High thermoelectric properties in full-Heusler X₂YZ alloys (Xâ€‰â€‰=â€‰â€‰Ca, Sr, and Ba; Yâ€‰â€‰=â€‰â€‰Au	1.3	6
139	Adjusting magnetic moments of Sc13 and Y13 clusters by doping different X atom (X = Na, Mg, Al, Si, P). International Journal of Quantum Chemistry, 2010, 110, 1573-1582.	1.0	5
140	First-Principles Study of Spontaneous Polarization in SbFeO₃. Journal of the Physical Society of Japan, 2012, 81, 074702.	0.7	5
141	Ground State Structures, Electronic and Magnetic Properties of Sc_nFe (n=2â€“10) Clusters. Chinese Journal of Chemistry, 2012, 30, 905-913.	2.6	5
142	Novel (1 Ã— 1)-reconstructions and native defects of TiO2 anatase (101) surface. Applied Surface Science, 2017, 405, 205-208.	3.1	5
143	Large enhanced conversion efficiency of perovskite solar cells by CsBr doping. Journal of Materials Science, 2017, 52, 13203-13211.	1.7	5
144	An unexpected interaction between a H2O2 molecule and anatase TiO2(101) surface. Applied Surface Science, 2019, 493, 926-932.	3.1	5

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145	First-principles investigation of the electronic structures and Seebeck coefficients of PbTe/SrTe interfaces. Journal of Applied Physics, 2019, 125, 035107.	1.1	5
146	An ab initio investigation of boron nanotube in ringlike cluster form. Applied Physics Letters, 2010, 96, 131901.	1.5	4
147	Geometries, stabilities, and electronic properties of YnSi (n=2â€“14) clusters: Density-functional theory investigations. Computational Materials Science, 2011, 50, 2167-2171.	1.4	4
148	Density-Functional Study of the Electronic Structure and Optical Properties of Transparent Conducting Oxides In4Sn3O12 and In4Ge3O12. Journal of Electronic Materials, 2011, 40, 1501-1505.	1.0	4
149	First-principles study of the (001) and (110) surfaces of superhard ReB2. Thin Solid Films, 2012, 520, 4951-4955.	0.8	4
150	Spin thermoelectric effects in Rashba quantum dots system. Solid State Communications, 2013, 159, 98-101.	0.9	4
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