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	Distinct transport behaviors and electronic structures in Heusler alloys CoFeCrGa and CoFeCrAl. Journal of Magnetism and Magnetic Materials, 2021, 517, 167383.	1.0	4
2	Thermoelectric properties of S-substituted BiCuSeO at O sites: First-principles study. Science China: Physics, Mechanics and Astronomy, 2020, 63, 1.	2.0	4
3	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
4	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
5	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
6	Tunable Magnetic Anisotropy and Dzyaloshinskii-Moriya Interaction in an Ultrathin van der Waals Fe3GeTe2/In2Se3 Heterostructure. Frontiers in Physics, 2020, 8, .	1.0	10
7	Ferroelectrically tunable magnetism in BiFeO3/BaTiO3 heterostructure revealed by the first-principles calculations. Journal of Advanced Research, 2020, 24, 371-377.	4.4	7
8	Stabilization of Skyrmions in a Nanodisk Without an External Magnetic Field. Physical Review Applied, 2020, 13, .	1.5	8
9	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
10	InTeI: a novel wide-bandgap 2D material with desirable stability and highly anisotropic carrier mobility. Nanoscale, 2020, 12, 5888-5897.	2.8	39
11	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
12	An unexpected interaction between a H2O2 molecule and anatase TiO2(101) surface. Applied Surface Science, 2019, 493, 926-932.	3.1	5
13	High thermoelectric properties in full-Heusler X₂YZ alloys (Xâ€‰â€‰=â€‰â€‰Ca, Sr, and Ba; Yâ€‰â€‰=â€‰â€‰A	1.3	6
14	Transition metal embedded C₃N monolayers as promising catalysts for the hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2019, 21, 20432-20441.	1.3	32
15	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
16	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
17	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
18	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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19	First-principles investigation of the electronic structures and Seebeck coefficients of PbTe/SrTe interfaces. Journal of Applied Physics, 2019, 125, 035107.	1.1	5
20	Tuning the magnetism of two-dimensional hematene by ferroelectric polarization. Physical Chemistry Chemical Physics, 2019, 21, 12301-12309.	1.3	16
21	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
22	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
23	Ab initio simulation studies on the room-temperature ferroelectricity in two-dimensional Î² -phase GeS. Applied Physics Letters, 2019, 114, .	1.5	72
24	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
25	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
26	Magneto-Seebeck effect in Co₂FeAl/MgO/Co₂FeAl: first-principles calculations. Physical Chemistry Chemical Physics, 2019, 21, 5803-5812.	1.3	12
27	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
28	Î³-GeSe: A two-dimensional ferroelectric material with doping-induced ferromagnetism. Applied Physics Letters, 2019, 115, .	1.5	41
29	Half-filled bands from Bi-Se sigma bonds and Bi 6s â€œlone-pairsâ€•induced superior thermoelectric properties of Bi/Cl codoped SnSe. Journal of Alloys and Compounds, 2019, 772, 1061-1066.	2.8	3
30	Isoelectronic indium doping for thermoelectric enhancements in BiCuSeO. Applied Surface Science, 2019, 473, 985-991.	3.1	22
31	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
32	Robust manipulation of magnetism in LaAO₃/BaTiO₃ (A = Fe, Mn) Tj ETQq0 0 0 rgBT /Overlock	1.0	10
33	C3N monolayers as promising candidates for NO2 sensors. Sensors and Actuators B: Chemical, 2018, 266, 664-673.	4.0	172
34	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
35	Optimizing the electrical transport properties of InBr via pressure regulation. Journal of Applied Physics, 2018, 124, .	1.1	3
36	Thermoelectric properties of monolayer Sb2Te3. Journal of Applied Physics, 2018, 124, .	1.1	42

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37	Pressure effect on the electronic structure and thermoelectric properties of Î±-MgAgSb. Computational Materials Science, 2018, 155, 450-456.	1.4	9
38	Engineering electrical transport in Î±-MgAgSb to realize high performances near room temperature. Physical Chemistry Chemical Physics, 2018, 20, 16729-16735.	1.3	15
39	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
40	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
41	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
42	Improvement of Thermoelectricity Through Magnetic Interactions in Layered Cr₂Ge₂Te₆. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1800172.	1.2	9
43	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
44	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
45	Novel (1 Ã— 1)-reconstructions and native defects of TiO2 anatase (101) surface. Applied Surface Science, 2017, 405, 205-208.	3.1	5
46	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
47	Enhanced piezoelectricity of monolayer phosphorene oxides: a theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 27508-27515.	1.3	27
48	Optimum electronic structures for high thermoelectric figure of merit within several isotropic elastic scattering models. Scientific Reports, 2017, 7, 10104.	1.6	8
49	Ag-Mg antisite defect induced high thermoelectric performance of Î±-MgAgSb. Scientific Reports, 2017, 7, 2572.	1.6	28
50	Large enhanced conversion efficiency of perovskite solar cells by CsBr doping. Journal of Materials Science, 2017, 52, 13203-13211.	1.7	5
51	The driving force for forming Asâ€“As bonding and its effect on the electronic structures and the thermoelectric properties of Zintl Ca5M2As6 (M = Sn, Ga). RSC Advances, 2017, 7, 14262-14271.	1.7	1
52	Hf/Sb co-doping induced a high thermoelectric performance of ZrNiSn: First-principles calculation. Scientific Reports, 2017, 7, 14590.	1.6	16
53	Antibonding Holes Induce Good Thermoelectric Properties ofp-type Ca5Ga2As6. Journal of the Physical Society of Japan, 2017, 86, 074707.	0.7	1
54	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></m on its ultralow thermal conductivity. Physical Review B, 2017, 96, .	1.1	52

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55	Electronic structure and thermoelectric transport properties of the golden Th2S3-type Ti2O3 under pressure. AIP Advances, 2016, 6, .	0.6	0
56	Optimizing the Dopant and Carrier Concentration of Ca5Al2Sb6 for High Thermoelectric Efficiency. Scientific Reports, 2016, 6, 29550.	1.6	10
57	Mg₂Sn: a potential mid-temperature thermoelectric material. RSC Advances, 2016, 6, 48728-48736.	1.7	20
58	A graphene-coupled Bi₂WO₆ nanocomposite with enhanced photocatalytic performance: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 14113-14121.	1.3	27
59	The unusual chemical bonding and thermoelectric properties of a new type Zintl phase compounds Ba3Al2As4. Solid State Communications, 2016, 237-238, 28-33.	0.9	3
60	Origin of high thermoelectric performance of FeNb1â^'xZr/HfxSb1â^'ySny alloys: A first-principles study. Scientific Reports, 2016, 6, 33120.	1.6	20
61	Lithium Doping to Enhance Thermoelectric Performance of MgAgSb with Weak Electronâ€“Phonon Coupling. Advanced Energy Materials, 2016, 6, 1502269.	10.2	122
62	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
63	The electronic structure and thermoelectric properties of BiTl9Te6 and SbTl9Te6: First-principles calculations. Journal of Applied Physics, 2015, 118, 235703.	1.1	1
64	Tuning magnetism by biaxial strain in native ZnO. Physical Chemistry Chemical Physics, 2015, 17, 16536-16544.	1.3	19
65	The ground-state structure and physical properties of ReB₃ and IrB₃ predicted from first principles. RSC Advances, 2015, 5, 25919-25928.	1.7	16
66	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
67	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
68	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
69	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
70	A class of rare antiferromagnetic metallic oxides: double perovskite AMn₃V₄O₁₂ (A = Na⁺, Ca²⁺, and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 12717-12721.	1.3	6
71	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
72	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

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73	Optical and electrical properties of textured sulfur-hyperdoped silicon: a thermal annealing study. Journal of Materials Science, 2015, 50, 3391-3398.	1.7	12
74	Electronic structure and thermoelectric properties of the Zintl compounds Sr₅Al₂Sb₆ and Ca₅Al₂Sb₆: first-principles study. RSC Advances, 2015, 5, 50720-50728.	1.7	10
75	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
76	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
77	Enhanced photocatalytic H2-production activity of bicomponent NiO/TiO2 composite nanofibers. Journal of Colloid and Interface Science, 2015, 449, 115-121.	5.0	136
78	ç»“æž„æœçº¢ç¨‹åºCALYPSOåœ¨æ–°åž‹è¶…ç¡¬æœ™æŽ¢ç´¢æ–¹é¢çš„å¹”ç”¨. Chinese Science Bulletin, 2015, 60, 2601-2607.	0.7	0
79	Nitrogen Vacancies and Oxygen Substitution of Ta₃N₅: First-Principles Investigation. Journal of the Physical Society of Japan, 2014, 83, 114707.	0.7	17
80	Electronic structure and thermoelectric performance of Zintl compound Sr3GaSb3: A first-principles study. Applied Physics Letters, 2014, 104, .	1.5	11
81	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
82	Electronic structure and thermoelectric properties of orthorhombic SrLiAs. Journal of Applied Physics, 2014, 116, 033705.	1.1	6
83	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
84	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
85	Improved thermoelectric performance of CuGaTe2 with convergence of band valleys: a first-principles study. RSC Advances, 2014, 4, 28714.	1.7	27
86	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
87	Predicted boron-carbide compounds: A first-principles study. Journal of Chemical Physics, 2014, 140, 224704.	1.2	33
88	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
89	A key factor improving the thermoelectric properties of Zintl compounds A5M2Pn6 (A=Ca, Sr, Ba;) Tj ETQq1 1 0.784314 rgBT /Overlo	1.4	8
90	Giant magnetic moments of Pd-doped manganese clusters. Molecular Physics, 2013, 111, 951-957.	0.8	0

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91	A new hard phase of ReB4 predicted from first principles. Journal of Alloys and Compounds, 2013, 573, 20-26.	2.8	34
92	Electronic Structure and Thermoelectric Properties of ZnO Single-Walled Nanotubes and Nanowires. Journal of Physical Chemistry C, 2013, 117, 21037-21042.	1.5	19
93	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
94	Predicted crystal structures of molybdenum under high pressure. Journal of Alloys and Compounds, 2013, 556, 116-120.	2.8	15
95	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
96	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
97	Phase Stability and Elastic Properties of Chromium Borides with Various Stoichiometries. ChemPhysChem, 2013, 14, 1245-1255.	1.0	23
98	Spin thermoelectric effects in Rashba quantum dots system. Solid State Communications, 2013, 159, 98-101.	0.9	4
99	Tuning the Magnetism by CO Adsorption in Graphene-Like ZnO with Defect. Journal of the Physical Society of Japan, 2013, 82, 064702.	0.7	2
100	Investigation on three-photon-absorption fitting method and three-photon-absorption-induced optical stabilication effect of a fluorene derivative. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 017801.	0.2	0
101	First-Principles Investigation of Hexagonal WB2 Surfaces. Journal of the Physical Society of Japan, 2012, 81, 044712.	0.7	3
102	Three-photon-absorption-induced optical stabilization effects in a bifluorenylidene derivative. Optics Express, 2012, 20, 14596.	1.7	3
103	Electronic structure and thermoelectric performance of Zintl compound Ca5Ga2As6. Journal of Materials Chemistry, 2012, 22, 20284.	6.7	24
104	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
105	First-Principles Study of Spontaneous Polarization in SbFeO₃. Journal of the Physical Society of Japan, 2012, 81, 074702.	0.7	5
106	New Crystal Structures of IrB and IrB₂: First-Principles Calculations. Journal of Physical Chemistry C, 2012, 116, 21961-21966.	1.5	19
107	Possible Origin of Ferromagnetism in an Undoped ZnO d0 Semiconductor. Journal of Physical Chemistry C, 2012, 116, 9709-9715.	1.5	50
108	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

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109	Structural, Electronic, and Thermoelectric Properties of InSe Nanotubes: First-Principles Calculations. Journal of Physical Chemistry C, 2012, 116, 3956-3961.	1.5	14
110	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
111	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
112	First-principles study of the (001) and (110) surfaces of superhard ReB2. Thin Solid Films, 2012, 520, 4951-4955.	0.8	4
113	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
114	Electronic structure and low temperature thermoelectric properties of In₂₄ M₈ O₄₈ (M = Ge⁴⁺, Sn⁴⁺, Ti⁴⁺, and) Tj ETQq0 0 1 rgBT /Overlock 10	1.5	8
115	Geometries, Stabilities and Electronic Properties of Au₁₂M (M=Na, Mg, Al, Si, P, S,) Tj ETQq1 1 0.784314 rgBT	2.2	8
116	Vacancy and Oxygen Substitution for Nitrogen-Induced Structural Stability of Ta₂N₃. Journal of Physical Chemistry C, 2011, 115, 3129-3135.	1.5	12
117	The electronic and magnetic properties of MnScN(Nâ€‰=â€‰2â€“10) clusters. Molecular Physics, 2011, 109, 1957-1965.	0.8	6
118	Phase Stability and Physical Properties of Manganese Borides: A First-Principles Study. Journal of Physical Chemistry C, 2011, 115, 21429-21435.	1.5	60
119	Crystal structure, electronic structure, and thermoelectric properties of Ca5Al2Sb6. Journal of Materials Chemistry, 2011, 21, 12497.	6.7	38
120	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
121	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
122	Firstâ€principles study of CrB₄ as a high shear modulus compound. Physica Status Solidi - Rapid Research Letters, 2011, 5, 13-15.	1.2	25
123	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
124	Giant magnetic moment of the coreâ€shell Co₁₃@Mn₂₀ clusters: Firstâ€principles calculations. Journal of Computational Chemistry, 2011, 32, 2474-2478.	1.5	13
125	Structural, electronic and magnetic properties of GdSi (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 117 Td (xmlns:mml= clusters: A density functional study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 1120-1127.	0.9	32
126	First-principles study of the elastic properties of and alloys. Solid State Communications, 2011, 151, 238-241.	0.9	25

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127	Pressure-induced phase transition of tantalum mononitride. Thin Solid Films, 2011, 519, 3954-3958.	0.8	14
128	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
129	Thermoelectric properties of Heusler-type compound Fe2V1â^'xNbxAl. Journal of Applied Physics, 2011, 110, 013530.	1.1	9
130	First-principles study of the electronic structure and optical properties of Ce-doped ZnO. Journal of Applied Physics, 2011, 109, .	1.1	55
131	Pressure induced structural phase transition of OsB2: First-principles calculations. Journal of Solid State Chemistry, 2010, 183, 915-919.	1.4	12
132	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
133	First-principles simulations of dissociated and molecular hydrogen adsorption on silicon oxide clusters. Computational and Theoretical Chemistry, 2010, 941, 71-77.	1.5	2
134	First-principles study of W, WN, WN₂, and WN₃. Physica Status Solidi (B): Basic Research, 2010, 247, 54-58.	0.7	19
135	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
136	An ab initio investigation of boron nanotube in ringlike cluster form. Applied Physics Letters, 2010, 96, 131901.	1.5	4
137	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
138	Investigation of osmium carbides with various stoichiometries: First-principles calculations. Journal of Applied Physics, 2010, 107, .	1.1	26
139	First-principles study of the structural, elastic, and electronic properties of C₂₀, C₁₂B₈, and C₁₂N₈. Journal of Physics Condensed Matter, 2010, 22, 175505.	0.7	0
140	First principles studies of phase stability, electronic and elastic properties in BBi compound. Computational Materials Science, 2010, 47, 968-972.	1.4	27
141	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
142	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
143	Structural transition of Li3N under high pressure: A first-principles study. Solid State Communications, 2009, 149, 612-615.	0.9	14
144	Pressure-induced structural transition in PuTe. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 1693-1696.	0.9	7

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145	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></mml:msub></mml:math> 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></mml:msub></mml:math> from first-principles calculations. Physical Review B, 2010, 82, 2880-2886.	1.4	47
146	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
147	A hard semiconductor OsN₄ with high elastic constant c₄₄. Physica Status Solidi - Rapid Research Letters, 2009, 3, 272-274.	1.2	9
148	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
149	First-principles study of zinc-blende to rocksalt phase transition in BP and BAs. Computational Materials Science, 2009, 44, 1386-1389.	1.4	24
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151	Structural and electronic properties of ZnO under high pressure. Journal of Alloys and Compounds, 2009, 476, 306-310.	2.8	42
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