Ponnaih Ravindran

List of Publications by Year
in descending order

96 papers	6,449 citations	101496 36 h-index	62565 80 g-index
97 all docs	97 docs citations	97 times ranked	6452 citing authors

#	Article	IF	Citations
1	Density functional theory for calculation of elastic properties of orthorhombic crystals: Application to TiSi2. Journal of Applied Physics, 1998, 84, 4891-4904.	1.1	1,565
2	Theoretical investigation of magnetoelectric behavior inBiFeO3. Physical Review B, 2006, 74, .	1.1	582
3	Electronic structure, bonding, and ground-state properties of AlB_{2}-type transition-metal diborides. Physical Review B, 2001, 63, .	1.1	436
4	Electronic structure and optical properties ofZnX(X=O,S, Se, Te): A density functional study. Physical Review B, 2007, 75, .	1.1	225
5	Phase stability, electronic structure, and optical properties of indium oxide polytypes. Physical Review B, 2007, 76, .	1.1	194
6	Pressure-Induced Structural Transitions inMgH2. Physical Review Letters, 2002, 89, 175506.	2.9	186
7	Large magnetocrystalline anisotropy in bilayer transition metal phases from first-principles full-potential calculations. Physical Review B, 2001, 63, .	1.1	182
8	Energetics of intrinsic defects and their complexes in ZnO investigated by density functional calculations. Physical Review B, 2011, 83, .	1.1	162
9	Electronic structure, chemical bonding, and optical properties of ferroelectric and antiferroelectricNaNO2. Physical Review B, 1999, 59, 1776-1785.	1.1	160
10	Detailed electronic structure studies on superconductingMgB2and related compounds. Physical Review B, 2001, 64, .	1.1	159
11	Structural stability and pressure-induced phase transitions inMgH2. Physical Review B, 2006, 73, .	1.1	154
12	Magnetic, optical, and magneto-optical properties of MnX(X=As, Sb, or Bi) from full-potential calculations. Physical Review B, 1999, 59, 15680-15693.	1.1	126
13	Pressure-induced phase of NaAlH4: A potential candidate for hydrogen storage?. Applied Physics Letters, 2003, 82, 2257-2259.	1.5	112
14	Theoretical Investigations on the Chemical Bonding, Electronic Structure, And Optical Properties of the Metalâ^'Organic Framework MOF-5. Inorganic Chemistry, 2010, 49, 10283-10290.	1.9	112
15	Itinerant metamagnetism and possible spin transition in LaCoO[sub 3] by temperature/hole doping. Journal of Applied Physics, 2002, 91, 291.	1.1	108
16	Ground-state and excited-state properties ofLaMnO3from full-potential calculations. Physical Review B, 2002, 65, .	1.1	108
17	Correlation between electronic structure, mechanical properties and phase stability in intermetallic compounds. Bulletin of Materials Science, 1997, 20, 613-622.	0.8	107
18	Coulomb correlation effects in zinc monochalcogenides. Journal of Applied Physics, 2006, 100, 043709.	1.1	86

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19	Optical properties of monoclinic SnI2from relativistic first-principles theory. Physical Review B, 1997, 56, 6851-6861.	1.1	82
20	Tailoring the Electronic Band Gap and Band Edge Positions in the C₂N Monolayer by P and As Substitution for Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2017, 121, 22216-22224.	1.5	80
21	Electronic structure and optical properties of ZnSiO3 and Zn2SiO4. Journal of Applied Physics, 2009, 106, .	1.1	75
22	High hydrogen content complex hydrides: A density-functional study. Applied Physics Letters, 2006, 89, 071906.	1.5	68
23	Ab initio investigations on the crystal structure, formation enthalpy, electronic structure, chemical bonding, and optical properties of experimentally synthesized isoreticular metalâ€“organic framework-10 and its analogues: M-IRMOF-10 (M = Zn, Cd, Be, Mg, Ca, Sr and Ba). RSC Advances, 2012, 2, 1618-1631.	1.7	63
24	Violation of the Minimum H-H Separation "Rule" for Metal Hydrides. Physical Review Letters, 2002, 89, 106403.	2.9	62
25	Electronic structure of multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BiFeO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> related compounds: Electron energy loss spectroscopy and density functional study. Physical Review B, 2010, 82, .	1.1	55
26	Graphene decorated with Fe nanoclusters for improving the hydrogen sorption kinetics of MgH₂ â€“ experimental and theoretical evidence. Catalysis Science and Technology, 2016, 6, 261-268.	2.1	54
27	Influence of hydrogen and halogen adsorption on the photocatalytic water splitting activity of C2N monolayer: A first-principles study. Carbon, 2019, 141, 50-58.	5.4	54
28	Potential hydrogen storage materials from metal decorated 2D-C₂N: an ab initio study. Physical Chemistry Chemical Physics, 2019, 21, 25311-25322.	1.3	53
29	Structural stability of BeH2 at high pressures. Applied Physics Letters, 2004, 84, 34-36.	1.5	51
30	Design of Potential Hydrogen-Storage Materials Using First-Principle Density-Functional Calculations. Crystal Growth and Design, 2004, 4, 471-477.	1.4	51
31	Short hydrogen-hydrogen separation inRNiInH1.333(R=La,Ce, Nd). Physical Review B, 2003, 67, .	1.1	47
32	Magneticâ€Instabilityâ€Induced Giant Magnetoelectric Coupling. Advanced Materials, 2008, 20, 1353-1356.	11.1	47
33	Enhanced Photocatalytic Water Splitting in a C₂N Monolayer by Câ€Site Isoelectronic Substitution. ChemPhysChem, 2017, 18, 1526-1532.	1.0	46
34	Two-Dimensional CdX/C₂N (X = S, Se) Heterostructures as Potential Photocatalysts for Water Splitting: A DFT Study. ACS Omega, 2020, 5, 23762-23768.	1.6	45
35	Electronic structure, phase stability, equation of state, and pressure-dependent superconducting properties ofZr3Al. Physical Review B, 1994, 50, 668-678.	1.1	40
36	Formation of an intermediate band in isoreticular metalâ€“organic framework-993 (IRMOF-993) and metal-substituted analogues M-IRMOF-993. Journal of Materials Chemistry, 2012, 22, 16324.	6.7	37

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37	Sign reversal of the orbital moment via ligand states. Physical Review B, 2001, 63, .	1.1	35
38	Hydrides as materials for semiconductor electronics. Philosophical Magazine, 2008, 88, 2461-2476.	0.7	33
39	Modeling of hydrogen storage materials by density-functional calculations. Journal of Power Sources, 2006, 159, 88-99.	4.0	32
40	Structural and electronic properties of transparent conducting delafossite: a comparison between the AgBO₂ and CuBO₂ families (BA= Al, Ga, In and Sc, Y). RSC Advances, 2015, 5, 1366-1377.	1.7	32
41	Novel High Pressure Phases of Î²-AlH3: A Density-Functional Study. Chemistry of Materials, 2008, 20, 5997-6002.	3.2	31
42	Influence of Crystal Structure of Bulk Phase on the Stability of Nanoscale Phases: Investigation on MgH₂ Derived Nanostructures. Journal of Physical Chemistry C, 2012, 116, 18965-18972.	1.5	30
43	Ab-initio studies on Li doping, Li-pairs, and complexes between Li and intrinsic defects in ZnO. Journal of Applied Physics, 2012, 111, .	1.1	29
44	Large Negative Thermal Expansion Induced by Synergistic Effects of Ferroelectrostriction and Spin Crossover in PbTiO₃-Based Perovskites. Chemistry of Materials, 2019, 31, 1296-1303.	3.2	29
45	Collective ionic motion in oxide fast-ion-conductors. Physical Chemistry Chemical Physics, 2004, 6, 3052-3055.	1.3	28
46	MgH₂ in Carbon Scaffolds: A Combined Experimental and Theoretical Investigation. Journal of Physical Chemistry C, 2012, 116, 21139-21147.	1.5	28
47	Effect of oxygen stoichiometry on spin, charge, and orbital ordering in manganites. Physical Review B, 2004, 69, .	1.1	25
48	Spin- and charge-ordering in oxygen-vacancy-ordered mixed-valenceSr4Fe4O11. Physical Review B, 2006, 74, .	1.1	24
49	Electronic structure, phase stability, and chemical bonding inTh2AlandTh2AlH4. Physical Review B, 2002, 65, .	1.1	23
50	Prediction of large polar Kerr rotation in the Heusler-related alloys AuMnSb and AuMnSn. Applied Physics Letters, 2003, 82, 2862-2864.	1.5	22
51	Search for metal hydrides with short hydrogenâ€“hydrogen separation:â€‚Ab initiocalculations. Physical Review B, 2004, 70, .	1.1	21
52	Site preference of hydrogen in metal, alloy, and intermetallic frameworks. Europhysics Letters, 2005, 72, 569-575.	0.7	19
53	Theoretical modeling of hydrogen storage materials: Prediction of structure, chemical bond character, and high-pressure behavior. Journal of Alloys and Compounds, 2005, 404-406, 377-383.	2.8	18
54	Spin, charge, and orbital ordering in the ferrimagnetic insulatorYBaMn2O5. Physical Review B, 2002, 65, .	1.1	17

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55	Hydride electronics. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 3538-3544.	0.8	17
56	Prediction of crystal structure, lattice dynamical, and mechanical properties of CaB2H2. International Journal of Hydrogen Energy, 2011, 36, 10149-10158.	3.8	16
57	Prediction of structural, lattice dynamical, and mechanical properties of CaB2. RSC Advances, 2012, 2, 11687.	1.7	15
58	Thermal, electronic and thermoelectric properties of TiNiSn and TiCoSb based quaternary half Heusler alloys obtained fromab initiocalculations. Sustainable Energy and Fuels, 2020, 4, 895-910.	2.5	15
59	Theoretical and experimental investigation on structural, electronic and magnetic properties of layered Mn₅O₈. Physical Chemistry Chemical Physics, 2016, 18, 27885-27896.	1.3	14
60	Absence of a pressure-induced structural phase transition inTi3Alup to 25 GPa. Physical Review B, 2000, 63, .	1.1	13
61	Earth-abundant nontoxic direct band gap semiconductors for photovoltaic applications by ab-initio simulations. Solar Energy, 2019, 190, 350-360.	2.9	11
62	Density Functional Theory Studies of Spin, Charge, and Orbital Ordering in YBaT₂O₅(T = Mn, Fe, Co). Inorganic Chemistry, 2008, 47, 6608-6620.	1.9	10
63	Electronic and Magnetic Structures of Hole Doped Trilayer La_{4â€“x}Sr_xNi₃O₈from First-Principles Calculations. Inorganic Chemistry, 2016, 55, 11898-11907.	1.9	9
64	Metamagnetism stabilized giant magnetoelectric coupling in ferroelectric xBaTiO3â€“(1 â^' x)BiCoO3 solid solution. Physical Chemistry Chemical Physics, 2018, 20, 7021-7032.	1.3	8
65	Amphoteric behavior of hydrogen (H⁺¹ and H^{â^'1}) in complex hydrides from van der Waals interaction-including ab initio calculations. Journal of Materials Chemistry A, 2019, 7, 6228-6240.	5.2	7
66	Te doped indium (II) selenide photocatalyst for water splitting: A first principles study. AIP Conference Proceedings, 2017, , .	0.3	6
67	Phase Stability, Phase Mixing, and Phase Separation in Fluorinated Alkaline Earth Hydrides. Journal of Physical Chemistry C, 2017, 121, 21806-21820.	1.5	6
68	Investigation of Electronic Structure and Electrochemical Properties of Na2MnSiO4 as a Cathode Material for Na Ion Batteries. Journal of Physical Chemistry C, 2021, 125, 25968-25982.	1.5	6
69	Antiperovskite materials as promising candidates for efficient tandem photovoltaics: First-principles investigation. Materials Science in Semiconductor Processing, 2022, 147, 106727.	1.9	6
70	First principles prediction of the ground state crystal structures of antiperovskite compounds A3PN (A= Be, Mg, Ca, Sr, Ba and Zn). Materials Today: Proceedings, 2019, 8, 294-300.	0.9	5
71	Zinc substituted MgH2 - a potential material for hydrogen storage applications. International Journal of Hydrogen Energy, 2019, 44, 13632-13646.	3.8	5
72	Role of W-site substitution on mechanical and electronic properties of cubic tungsten carbide. Journal of Physics Condensed Matter, 2020, 32, 145701.	0.7	5

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73	Structural phase stability in fluorinated calcium hydride. AIP Conference Proceedings, 2017, , .	0.3	3
74	Phosphorene-AsP heterostructure as a potential excitonic solar cell material - A first principles study. AIP Conference Proceedings, 2018, , .	0.3	3
75	Ti4+ substituted magnesium hydride as promising material for hydrogen storage and photovoltaic applications. AIP Conference Proceedings, 2019, , .	0.3	3
76	First-principles density-functional calculations on HCr3O8: An exercise to better understand the ACr3O8(A = alkali metal) family. Journal of Electroceramics, 2006, 17, 15-20.	0.8	2
77	The search for novel hydrogen storage materials: a theoretical approach. International Journal of Nuclear Hydrogen Production and Applications, 2009, 2, 137.	0.2	2
78	Chemical bonding analysis on amphoteric hydrogen â€“ alkaline earth ammine borohydrides. AIP Conference Proceedings, 2018, , .	0.3	2
79	Comment on the paper titledâ€œTwo-dimensional Sc2C: A reversible and high capacity hydrogen storage material predicted by first-principles calculationsâ€•by Hu etÂal., International Journal of Hydrogen Energy, 2014; 69, 1â€“4. International Journal of Hydrogen Energy, 2020, 45, 7254-7256.	3.8	2
80	Revealing the optoelectronic properties of tin-based vacancy ordered double perovskites: K2SnBr6 and Rb2SnBr6. AIP Conference Proceedings, 2021, , .	0.3	2
81	Effect of multinary substitution on electronic and transport properties of TiCoSb based half-Heusler alloys. AIP Conference Proceedings, 2018, , .	0.3	1
82	A first principle study on iron substituted LiNi (BO3) to use as cathode material for Li-ion batteries. AIP Conference Proceedings, 2018, , .	0.3	1
83	Giant Magnetoelectric Coupling in Multiferroic PbTi_{1â€“x}V_xO₃ from Density Functional Calculations. ACS Omega, 2019, 4, 16743-16755.	1.6	1
84	Effect of Electron Doping on the Crystal Structure and Physical Properties of an n = 3 Ruddlesdenâ€“Popper Compound La₄Ni₃O₁₀. ACS Applied Electronic Materials, 2021, 3, 2671-2684.	2.0	1
85	Unravelling the crystal structure and optoelectronic properties of C3H3MI3 (M = Sn, Pb) for solar cell applications. Solar Energy Materials and Solar Cells, 2021, 230, 111133.	3.0	1
86	Search for thermoelectrics with high figure of merit in half-Heusler compounds with multinary substitution. AIP Conference Proceedings, 2018, , .	0.3	0
87	Theoretical investigation of the magnetoelectric properties of Bi2NiTiO6. AIP Conference Proceedings, 2018, , .	0.3	0
88	Magnetoelectric properties of Pb free Bi2FeTiO6: A theoretical investigation. AIP Conference Proceedings, 2018, , .	0.3	0
89	Ab-initio modelling of new cathode material for Li-ion battery based on the Ti substituted Li2Fe(SO4)2. AIP Conference Proceedings, 2019, , .	0.3	0
90	Li-rich Li6MnxFe(1-x)S4 as cathode material for Li-ion battery. AIP Conference Proceedings, 2019, , .	0.3	0

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91	Theoretical investigation on the effect of multinary isoelectronic substitution on TiCoSb based half-Heusler alloys. AIP Conference Proceedings, 2019, , .	0.3	0
92	Effect of anionic and cationic substitutions on the magnetic property of hydrated Î±-MnO2. AIP Conference Proceedings, 2019, , .	0.3	0
93	Amphoteric behavior of hydrogen in bimetallic molecular like hydrides. AIP Conference Proceedings, 2019, , .	0.3	0
94	Ab-initio based thermodynamic study on Î±-NaMnO2 for Na-ion battery applications. AIP Conference Proceedings, 2019, , .	0.3	0
95	A promising cathode material with high Na content for Na-ion battery applications from ab-initio calculations. AIP Conference Proceedings, 2021, , .	0.3	0
96	Understanding the optoelectronic properties of interface between Cs2TiBr6 and TiO2 for solar cell applications. Materials Today Communications, 2022, 32, 103963.	0.9	0