Ponniah Vajeeston

List of Publications by Year
in descending order

121	4,033	136740	133063
papers	citations	32 h-index	59 g-index

126	126	126	4320
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Disorder-Induced Ordering in Gallium Oxide Polymorphs. Physical Review Letters, 2022, 128, 015704.	2.9	36
2	Operando XRD studies on Bi₂MoO₆ as anode material for Na-ion batteries. Nanotechnology, 2022, 33, 185402.	1.3	9
3	Thin films made by reactive sputtering of high entropy alloy FeCoNiCuGe: Optical, electrical and structural properties. Thin Solid Films, 2022, 744, 139083.	0.8	3
4	High entropy alloy CrFeNiCoCu sputter deposited films: Structure, electrical properties, and oxidation. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2022, 40, .	0.9	3
5	First-Principles Exploration into the Physical and Chemical Properties of Certain Newly Identified SnO₂ Polymorphs. ACS Omega, 2022, 7, 10382-10393.	1.6	13
6	Antifluorite-type Na₅FeO₄ as a low-cost, environment-friendly cathode with combined cationic/anionic redox activity for sodium ion batteries: a first-principles investigation. RSC Advances, 2022, 12, 17410-17421.	1.7	3
7	Superconducting and structural properties of the noncentrosymmetric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Re</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math> superconductor under high pressure. Physical Review B, 2022, 105, .	1.1	2
8	Structural stability and electronical properties of MoSe2 polymorphs: DFT. Materials Today: Proceedings, 2022, , .	0.9	1
9	Computational study on electronic and thermal stability of low energy indium oxide polytypes. Materials Today: Proceedings, 2022, , .	0.9	0
10	Cs2AgBiBr6 as a mixed anion perovskites for photovoltaic applications: A first-principle study. Materials Today: Proceedings, 2022, 64, 1783-1788.	0.9	1
11	Reaction induced multifunctional TiO2 rod/particle nanostructured materials for screen printed dye sensitized solar cells. Ceramics International, 2021, 47, 8094-8104.	2.3	4
12	The average and local structure of TiVCrNbD<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si47.svg"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math> (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 302 Td (xmlns:mml="http://www	3.8	33
13	In-depth first-principle study on novel MoS₂ polymorphs. RSC Advances, 2021, 11, 3759-3769.	1.7	13
14	Pressure-induced structural transition and huge enhancement of superconducting properties of single-crystal Fe0.99Ni0.01Se0.5Te0.5 unconventional superconductor. Journal of Materials Research, 2021, 36, 1624-1636.	1.2	1
15	TiO2 as a Photocatalyst for Water Splittingâ€"An Experimental and Theoretical Review. Molecules, 2021, 26, 1687.	1.7	114
16	Pressure-dependent modifications in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LaAu</mml:mi><mml:msub><mml:mi>Sb</mml:mi><mml:mi><mml:mi> charge density wave system. Physical Review B, 2021, 103, .	1.1	6
17	Vibrational properties of High Entropy Alloy based metal hydrides probed by inelastic neutron scattering. Journal of Alloys and Compounds, 2021, 877, 160320.	2.8	4
18	Pressure Dependence of Superconducting Properties, Pinning Mechanism, and Crystal Structure of the Fe_{0.99}Mn_{0.01}Se_{0.5}Te_{0.5}Superconductor. ACS Omega, 2021, 6, 30419-30431.	1.6	2

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19	Insights into Crystal Structure and Diffusion of Biphasic Na₂Zn₂TeO₆. ACS Applied Materials & Interfaces, 2020, 12, 28188-28198.	4.0	14
20	Carbon-dioxide as annealing atmosphere to retain the electrical properties of indium-tin oxide. Materials Letters, 2020, 276, 128195.	1.3	2
21	One-pot synthesis of cobaltâ€“rhenium nanoparticles taking the unusual Î²-Mn type structure. Nanoscale Advances, 2020, 2, 1850-1853.	2.2	5
22	Factors Determining Microporous Material Stability in Water: The Curious Case of SAPO-37. Chemistry of Materials, 2020, 32, 1495-1505.	3.2	15
23	Direct observation of reversible conversion and alloying reactions in a Bi₂(MoO₄)₃-based lithium-ion battery anode. Journal of Materials Chemistry A, 2019, 7, 17906-17913.	5.2	9
24	A combined deep inelastic neutron scattering and ab initio lattice dynamics study of the hydride anion dynamics and bonding in La₂LiHO₃ oxyhydride. Journal of Physics Communications, 2019, 3, 103002.	0.5	11
25	First-Principle Calculation of High Absorption-TlGaTe2 for Photovoltaic Application. Materials, 2019, 12, 2667.	1.3	1
26	Advances in the LiCl salt flux method and the preparation of phase pure La_{2â^'x}Nd_xLiHO₃ (0 â‰ x â‰ 2) oxyhydrides. Chemical Communications, 2019, 55, 3817-3820.	2.2	7
27	Nonhexagonal Na Sublattice Reconstruction in the Super-Ionic Conductor Na2Zn2TeO6: Insights from Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2019, 123, 4654-4663.	1.5	9
28	P2 Type Layered Solid-State Electrolyte Na₂Zn₂TeO₆: Crystal Structure and Stacking Faults. Journal of the Electrochemical Society, 2019, 166, A3830-A3837.	1.3	10
29	First-Principles Study of the Structural Stability and Dynamic Properties of Li2MSiO4 (M = Mn, Co, Ni) Polymorphs. Energies, 2019, 12, 224.	1.6	7
30	Anisotropy of the proton kinetic energy in ice Ih. Surface Science, 2019, 679, 174-179.	0.8	2
31	Ionic conductivity enhancement by particle size reduction in Li2FeSiO4. Materials Letters, 2018, 218, 313-316.	1.3	19
32	A first-principle study of the electronic, mechanical and optical properties of inorganic perovskite Cs2SnI6 for intermediate-band solar cells. Materials Letters, 2018, 218, 233-236.	1.3	61
33	Bandgap engineering in CsSnxPb(1â^'x)I3 and their influence on light absorption. Materials Letters, 2018, 218, 253-256.	1.3	11
34	Search for potential precursors for Si-atomic layer deposition â€“ A quantum chemical study. Materials Letters, 2018, 216, 189-192.	1.3	4
35	New Insights into Hydride Bonding, Dynamics, and Migration in La₂LiHO₃ Oxyhydride. Journal of Physical Chemistry Letters, 2018, 9, 353-358.	2.1	27
36	A first-principle investigation of the Li diffusion mechanism in the super-ionic conductor lithium orthothioborate Li3BS3 structure. Materials Letters, 2018, 219, 186-189.	1.3	9

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37	A first principle comparative study of the ionic diffusivity in LiAlO2 and NaAlO2 polymorphs for solid-state battery applications. Physical Chemistry Chemical Physics, 2018, 20, 9824-9832.	1.3	16
38	Operando investigations of lithiation and delithiation processes in a BiVO₄ anode material. Physical Chemistry Chemical Physics, 2018, 20, 29798-29803.	1.3	15
39	Hybrid Density Functional Study of Au2Cs2I6, Ag2GeBaS4, Ag2ZnSnS4, and AgCuPO4 for the Intermediate Band Solar Cells. Energies, 2018, 11, 3457.	1.6	5
40	Properties of Novel Non-Silicon Materials for Photovoltaic Applications: A First-Principle Insight. Materials, 2018, 11, 2006.	1.3	11
41	A promising high-efficiency photovoltaic alternative non-silicon material: A first-principle investigation. Scripta Materialia, 2018, 156, 134-137.	2.6	2
42	Lithium ionic conduction in composites of Li(BH4)0.75I0.25 and amorphous 0.75Li2SÂ·0.25P2S5 for battery applications. Electrochimica Acta, 2018, 278, 332-339.	2.6	35
43	A first-principle study of NaMPO4 (M = Mn, Fe, Co, Ni) possible novel structures as cathode materials for sodium-ion batteries: Structural and electrochemical characterisation. Materials Chemistry and Physics, 2018, 219, 212-221.	2.0	14
44	Computational Modeling of Novel Bulk Materials for the Intermediate-Band Solar Cells. ACS Omega, 2017, 2, 1454-1462.	1.6	26
45	Temperature induced transitions in La 4 (Co 1â^'x Ni x) 3 O 10+Î´ ; oxygen stoichiometry and mobility. Solid State Ionics, 2017, 305, 7-15.	1.3	10
46	First-principles study of the structural stability and electrochemical properties of Na₂MSiO₄ (M = Mn, Fe, Co and Ni) polymorphs. Physical Chemistry Chemical Physics, 2017, 19, 14462-14470.	1.3	31
47	Bismuth Vanadate and Molybdate: Stable Alloying Anodes for Sodium-Ion Batteries. Chemistry of Materials, 2017, 29, 2803-2810.	3.2	44
48	First-principles study of structural stability, dynamical and mechanical properties of Li₂FeSiO₄ polymorphs. RSC Advances, 2017, 7, 16843-16853.	1.7	32
49	Ab initio structure solution and thermal stability evaluation of a new Ca(<scp>ii</scp>) 3D coordination polymer using synchrotron powder X-ray diffraction data. CrystEngComm, 2017, 19, 5857-5863.	1.3	1
50	Chemical Structures of Specific Sodium Ion Battery Components Determined by Operando Pair Distribution Function and Xâ€ray Diffraction Computed Tomography. Angewandte Chemie - International Edition, 2017, 56, 11385-11389.	7.2	54
51	Chemical Structures of Specific Sodium Ion Battery Components Determined by Operando Pair Distribution Function and Xâ€ray Diffraction Computed Tomography. Angewandte Chemie, 2017, 129, 11543-11547.	1.6	5
52	How Crystallite Size Controls the Reaction Path in Nonaqueous Metal Ion Batteries: The Example of Sodium Bismuth Alloying. Chemistry of Materials, 2016, 28, 2750-2756.	3.2	113
53	Two New Series of Coordination Polymers and Evaluation of Their Properties by Density Functional Theory. Crystal Growth and Design, 2016, 16, 339-346.	1.4	6
54	Crystal structures of aluminum-based hydrides. Emerging Materials Research, 2015, 4, 192-217.	0.4	13

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55	On the Thermal Stability and Structures of Layered Double Hydroxides Mg_{1â€“x}Al_x(OH)₂(NO₃)_xÂ·mH₂O (0.18â€‰â‰¤â€‰xâ€‰â‰¤â€‰0.38). European Journal of Inorganic Chemistry, 2015, 2015, 1775-1788.	2.4	10
56	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
57	Revised electronic structure, Raman and IR studies of AB2H2and ABCH (A = Sr, Ba; B = Al, Ga; C = Si, Ge) phases. RSC Advances, 2014, 4, 22-31.	1.7	2
58	A quantum mechanically guided view of Cd-MOF-5 from formation energy, chemical bonding, electronic structure, and optical properties. Microporous and Mesoporous Materials, 2013, 175, 50-58.	2.2	34
59	Atomic layer deposition of lithium nitride and carbonate using lithium silylamide. RSC Advances, 2012, 2, 6315.	1.7	42
60	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
61	Prediction of structural, lattice dynamical, and mechanical properties of CaB2. RSC Advances, 2012, 2, 11687.	1.7	15
62	MgH₂ in Carbon Scaffolds: A Combined Experimental and Theoretical Investigation. Journal of Physical Chemistry C, 2012, 116, 21139-21147.	1.5	28
63	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
64	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
65	Properties of IRMOF-14 and its analogues M-IRMOF-14 (M = Cd, alkaline earth metals): electronic structure, structural stability, chemical bonding, and optical properties. Physical Chemistry Chemical Physics, 2012, 14, 4713.	1.3	45
66	Reply to â€œA comment on â€˜Prediction of crystal structure, lattice dynamical, and mechanical properties of CaB2H2â€™ by Vajeeston etÂal., Int J Hydrogen Energy, 36 (2011) 10149â€“10158â€• International Journal of Hydrogen Energy, 2012, 37, 2711-2712.	3.8	1
67	Phonon, IR, and Raman Spectra, NMR Parameters, and Elastic Constant Calculations for AlH₃ Polymorphs. Journal of Physical Chemistry A, 2011, 115, 10708-10719.	1.1	20
68	Synthesis, Crystal Structure, and Thermal Properties of the First Mixed-Metal and Anion-Substituted Rare Earth Borohydride LiCe(BH₄)₃Cl. Journal of Physical Chemistry C, 2011, 115, 23591-23602.	1.5	50
69	The crystal structure of the first borohydride borate, Ca3(BD4)3(BO3). Journal of Materials Chemistry, 2011, 21, 7188.	6.7	25
70	Stability enhancement by particle size reduction in AlH3. Journal of Alloys and Compounds, 2011, 509, S662-S666.	2.8	15
71	Nano-Phases of NaBH₄ and KBH₄. Journal of Nanoscience and Nanotechnology, 2011, 11, 1929-1934.	0.9	4
72	Prediction of crystal structure, lattice dynamical, and mechanical properties of CaB2H2. International Journal of Hydrogen Energy, 2011, 36, 10149-10158.	3.8	16

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73	Revisiting isoreticular MOFs of alkaline earth metals: a comprehensive study on phase stability, electronic structure, chemical bonding, and optical properties of Aâ€“IRMOF-1 (A = Be, Mg, Ca, Sr, Ba). Physical Chemistry Chemical Physics, 2011, 13, 10191.	1.3	53
74	Structural investigation and thermodynamical properties of alkali calcium trihydrides. Journal of Chemical Physics, 2010, 132, 114504.	1.2	10
75	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
76	Nanostructures of LiBH4: a density-functional study. Nanotechnology, 2009, 20, 275704.	1.3	23
77	Predicting New Materials for Hydrogen Storage Application. Materials, 2009, 2, 2296-2318.	1.3	9
78	Phase stability and pressure-induced structural transitions at zero temperature in ZnSiO₃and Zn₂SiO₄. Journal of Physics Condensed Matter, 2009, 21, 485801.	0.7	20
79	The search for novel hydrogen storage materials: a theoretical approach. International Journal of Nuclear Hydrogen Production and Applications, 2009, 2, 137.	0.2	2
80	Hydrides as materials for semiconductor electronics. Philosophical Magazine, 2008, 88, 2461-2476.	0.7	33
81	Structural Phase Stability Studies on MBeH₃ (M = Li, Na, K, Rb, Cs) from Density Functional Calculations. Inorganic Chemistry, 2008, 47, 508-514.	1.9	27
82	Crystal chemistry and metal-hydrogen bonding in anisotropic and interstitial hydrides of intermetallics of rare earth (R) and transition metals (T), RT₃ and R₂T₇. Zeitschrift FÃ¼r Kristallographie, 2008, 223, 674-689.	1.1	22
83	First-principles investigations of the MMgH3 (, Na, K, Rb, Cs) series. Journal of Alloys and Compounds, 2008, 450, 327-337.	2.8	50
84	Novel High Pressure Phases of Î²-AlH3: A Density-Functional Study. Chemistry of Materials, 2008, 20, 5997-6002.	3.2	31
85	Semiconducting hydrides. Europhysics Letters, 2008, 82, 17006.	0.7	23
86	Theoretical investigations on low energy surfaces and nanowires of MgH₂. Nanotechnology, 2008, 19, 275704.	1.3	40
87	Structure and bonding in BAlH5 (, Ca, Sr) from first-principle calculations. Journal of Alloys and Compounds, 2007, 433, 225-232.	2.8	31
88	A new series of high hydrogen content hydrogen-storage materialsâ€”A theoretical prediction. Journal of Alloys and Compounds, 2007, 446-447, 44-47.	2.8	21
89	Phase stability, electronic structure, and optical properties of indium oxide polytypes. Physical Review B, 2007, 76, .	1.1	194
90	Hydride electronics. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 3538-3544.	0.8	17

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91	Structural stability and pressure-induced phase transitions inMgH2. Physical Review B, 2006, 73, .	1.1	154
92	Modeling of hydrogen storage materials by density-functional calculations. Journal of Power Sources, 2006, 159, 88-99.	4.0	32
93	Structural phase stability and bonding behavior ofBAlH5(B=Mg,Ba)from first-principles calculations. Physical Review B, 2006, 73, .	1.1	22
94	High hydrogen content complex hydrides: A density-functional study. Applied Physics Letters, 2006, 89, 071906.	1.5	68
95	Structural Stability of Alkali Boron Tetrahydrides ABH4 (A: Li, Na, K, Rb, Cs) from First Principle Calculation.. ChemInform, 2005, 36, no.	0.1	0
96	First-principles investigations of aluminum hydrides:M3AlH6(M=Na,K). Physical Review B, 2005, 71, .	1.1	24
97	Structural stability, electronic structure, and magnetic properties of mixed-valenceACr3O8phases (A=Na, K, Rb). Physical Review B, 2005, 72, .	1.1	4
98	Reply to â€œComment on â€˜Structural stability and electronic structure for Li3AlH6â€™â€‰â€¦ Physical Review B, 2005, 71, .	1.1	12
99	Site preference of hydrogen in metal, alloy, and intermetallic frameworks. Europhysics Letters, 2005, 72, 569-575.	0.7	19
100	Structural stability of alkali boron tetrahydrides ABH4 (A = Li, Na, K, Rb, Cs) from first principle calculation. Journal of Alloys and Compounds, 2005, 387, 97-104.	2.8	126
101	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
102	Search for metal hydrides with short hydrogenâ€“hydrogen separation:â€‚Ab initiocalculations. Physical Review B, 2004, 70, .	1.1	21
103	Structural stability of BeH2 at high pressures. Applied Physics Letters, 2004, 84, 34-36.	1.5	51
104	Crystal Structure of KAlH4 from First Principle Calculations.. ChemInform, 2004, 35, no.	0.1	0
105	Spin, charge, and orbital orderings in oxides with dual-valent transition metal ions. Ceramics International, 2004, 30, 1993-1998.	2.3	6
106	Design of Potential Hydrogen-Storage Materials Using First-Principle Density-Functional Calculations. Crystal Growth and Design, 2004, 4, 471-477.	1.4	51
107	Effect of oxygen stoichiometry on spin, charge, and orbital ordering in manganites. Physical Review B, 2004, 69, .	1.1	25
108	Structural stability and electronic structure forLi3AlH6. Physical Review B, 2004, 69, .	1.1	40

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109	Chemical-bonding and high-pressure studies on hydrogen-storage materials. Computational Materials Science, 2004, 30, 349-357.	1.4	31
110	Crystal structure of KAlH4 from first principle calculations. Journal of Alloys and Compounds, 2004, 363, L8-L12.	2.8	44
111	Ground- and excited-state properties of inorganic solids from full-potential density-functional calculations. Journal of Solid State Chemistry, 2003, 176, 338-374.	1.4	10
112	Pressure-induced phase of NaAlH4: A potential candidate for hydrogen storage?. Applied Physics Letters, 2003, 82, 2257-2259.	1.5	112
113	Huge-pressure-induced volume collapse inLiAlH4and its implications to hydrogen storage. Physical Review B, 2003, 68, .	1.1	91
114	Short hydrogen-hydrogen separation inRNiInH1.333(R=La,Ce, Nd). Physical Review B, 2003, 67, .	1.1	47
115	Violation of the Minimum H-H Separation "Rule" for Metal Hydrides. Physical Review Letters, 2002, 89, 106403.	2.9	62
116	Electronic structure, phase stability, and chemical bonding inTh2AlandTh2AlH4. Physical Review B, 2002, 65, .	1.1	23
117	Pressure-Induced Structural Transitions inMgH2. Physical Review Letters, 2002, 89, 175506.	2.9	186
118	Antiferromagnetic vs. ferromagnetic interactions and spin-glass-like behavior in ruthenates. Solid State Communications, 2002, 124, 293-298.	0.9	13
119	Electronic structure, bonding, and ground-state properties of AlB_{2}-type transition-metal diborides. Physical Review B, 2001, 63, .	1.1	436
120	Detailed electronic structure studies on superconductingMgB2and related compounds. Physical Review B, 2001, 64, .	1.1	159
121	Electronic structure, phase stability, and cohesive properties ofTi2XAl(X=Nb,V,Zr). Physical Review B, 1999, 60, 15683-15690.	1.1	41