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High-pressure structural study of fluoro-perovskite CsCdF₃ up to 60 GPa: A combined experimental and theoretical study

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#	Paper	IF	Citations
39	High pressure structural stability of BaLiF ₃ . <i>Journal of Applied Physics</i> , 2011 , 110, 123505	2.5	18
38	Calculation of physical properties of the cubic perovskite-type oxide using the PP-PW method based on the DFT theory. <i>Solid State Communications</i> , 2011 , 151, 908-915	1.6	6
37	Structural, elastic, electronic, optical and thermal properties of cubic perovskite CsCdF ₃ under pressure effect. <i>EPJ Applied Physics</i> , 2011 , 53, 30101	1.1	6
36	Pressure dependent mechanical and thermodynamical properties of Hg _{0.91} Mn _{0.09} Te semiconductor. <i>European Physical Journal B</i> , 2011 , 79, 495-502	1.2	3
35	First-principles calculations on structural, elastic, electronic, optical and thermal properties of CsPbCl ₃ perovskite. <i>Physica B: Condensed Matter</i> , 2011 , 406, 1837-1843	2.8	44
34	Hybrid density-functional calculations of structural, elastic and electronic properties for a series of cubic perovskites CsMF ₃ (M = Ca, Cd, Hg, and Pb). <i>Computational Materials Science</i> , 2012 , 58, 101-112	3.2	20
33	DFT-BASED AB INITIO STUDY OF THE ELECTRONIC AND OPTICAL PROPERTIES OF CESIUM BASED FLUORO-PEROVSKITE CsMF ₃ (M = Ca AND Sr). <i>International Journal of Modern Physics B</i> , 2012 , 26, 1250199 ^{1.1}	1.1	9
32	Full-Potential Calculation of Structural, Electronic, and Thermodynamic Properties of Fluoroperovskite (text{ CsMF ₃ }) (M = Be and Mg). <i>International Journal of Thermophysics</i> , 2012 , 33, 2339-2350	2.1	2
31	Theoretical prediction of the structural, elastic, electronic, optical and thermal properties of the cubic perovskites CsXF ₃ (X=Ca, Sr and Hg) under pressure effect. <i>Solid State Sciences</i> , 2012 , 14, 903-913 ^{3.4}	3.4	19
30	Elastic, electronic and thermodynamic properties of fluoro-perovskite KZnF ₃ via first-principles calculations. <i>Applied Physics A: Materials Science and Processing</i> , 2012 , 106, 645-653	2.6	33
29	First-principles study of the structural, electronic and thermal properties of CaLiF ₃ . <i>Physica Scripta</i> , 2013 , 88, 035702	2.6	5
28	Structural, elastic, electronic and optical properties of CsMCl ₃ (M=Zn, Cd). <i>Physica B: Condensed Matter</i> , 2013 , 420, 15-23	2.8	26
27	Investigation of the structural, mechanical, dynamical and thermal properties of CsCaF ₃ and CsCdF ₃ . <i>Materials Research Express</i> , 2016 , 3, 045903	1.7	5
26	Shift of indirect to direct bandgap and thermoelectric response of the cubic BiScO ₃ via DFT-mBJ studies. <i>Materials Science in Semiconductor Processing</i> , 2016 , 49, 40-47	4.3	29
25	Calculated high-pressure structural properties, lattice dynamics and quasi particle band structures of perovskite fluorides KZnF ₃ , CsCaF ₃ and BaLiF ₃ . <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 315403 ^{1.8}	1.8	5
24	Structural, electronic and optical properties of CsPbX ₃ (X=Cl, Br, I) for energy storage and hybrid solar cell applications. <i>Journal of Alloys and Compounds</i> , 2017 , 705, 828-839	5.7	119
23	A theoretical study of perovskite CsXCl ₃ (X=Pb, Cd) within first principles calculations. <i>Physica B: Condensed Matter</i> , 2017 , 510, 60-73	2.8	20

22	Study of pressure variation effect on structural, opto-electronic, elastic, mechanical, and thermodynamic properties of SrLiF ₃ . <i>Physica B: Condensed Matter</i> , 2017 , 525, 60-69	2.8	8
21	High pressure structural stability of the Na-Te system. <i>AIP Advances</i> , 2018 , 8, 035123	1.5	
20	Electronic, thermoelectric and transport properties of cesium cadmium trifluoride: A DFT study. 2018 ,		
19	Optical properties of Mn ²⁺ doped CsCdF ₃ : A potential real-time and retrospective UV and X-ray dosimeter material. <i>Journal of Applied Physics</i> , 2019 , 125, 233102	2.5	3
18	DFT-focused estimation of mechanical, thermoelectric and thermodynamic properties of ACdF ₃ (A=K, Rb, Cs) fluoroperovskites. <i>International Journal of Modern Physics B</i> , 2019 , 33, 1950314	1.1	7
17	Effect of pressure on the order-disorder phase transitions of B cations in A ₂ B ₂ X ₆ perovskites. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019 , 75, 1034-1041	1.8	2
16	Ab Initio Study of the Mechanical, Thermal and Optoelectronic Properties of the Cubic CsBaF ₃ . <i>Acta Physica Polonica A</i> , 2015 , 128, 34-42	0.6	19
15	Incipient geometric lattice instability of cubic fluoroperovskites. <i>Physical Review B</i> , 2021 , 104,	3.3	2
14	Study on the thermoelectric properties of p-type doped CsCdF ₃ and CsHgF ₃ with quartic anharmonicity. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2022 , 428, 127946	2.3	0
13	First-principal investigations of electronic, structural, elastic and optical properties of the fluoroperovskite TL ₂ F ₃ (L = Ca, Cd) compounds for optoelectronic applications.. <i>RSC Advances</i> , 2022 , 12, 7002-7008	3.7	0
12	Insight into the exemplary structural, elastic, electronic and optical nature of GaBeCl and InBeCl: a DFT study.. <i>RSC Advances</i> , 2022 , 12, 8172-8177	3.7	1
11	Structural phase transitions and magnetic superexchange in MAgF perovskites at high pressure.. <i>Chemistry - A European Journal</i> , 2022 ,	4.8	
10	Pressure-induced elastic, mechanical and opto-electronic response of RbCdF ₃ : A comprehensive computational approach. <i>Journal of Physics and Chemistry of Solids</i> , 2022 , 165, 110642	3.9	1
9	First-principles calculations to investigate band gap of cubic BaThO ₃ with systematic isotropic external static pressure and its impact on structural, elastic, mechanical, anisotropic, electronic and optical properties. <i>Journal of Physics and Chemistry of Solids</i> , 2022 , 169, 110878	3.9	0
8	Ab-initio study of pressure influenced elastic, mechanical and optoelectronic properties of Cd _{0.25} Zn _{0.75} Se alloy for space photovoltaics. 2022 , 12,		0
7	Theoretical Investigations into the Different Properties of Al-Based Fluoroperovskite AlMF ₃ (M = Cr, B) Compounds by the TB-MBJ Potential Method. 2022 , 15, 5942		0
6	Computational investigation to explore the effects of metals (Mg, Ca, Sr) doping on phase transition, electronic band structure and their repercussions on optical, elastic and mechanical properties of BaThO ₃ . 2023 , 98, 015814		0
5	First principles computation of insulator/semiconductor/metal transition and its impact on structural, elastic, mechanical, anisotropic and optical properties of CsSrF ₃ under systematic static isotropic pressure. 1-19		0

- 4 Cubic to pseudo-cubic tetragonal phase transformation with Mg, Ca, and Be doping and its impact on optoelectronic, elastic and mechanical properties of SrHfO₃. **2023**, 177, 111279
- 3 Assimilation of electronic, elastic, mechanical, optical, and thermal profiles in metal halide perovskite CsPbCl₃, for optoelectronic applications. **2023**, 35, e00804
- 2 Predicting structural, optoelectronic and mechanical properties of germanium based AGeF₃ (A = Ga and In) halides perovskites using the DFT computational approach. **2023**, 55,
- 1 Ab initio study of fundamental properties of ACdX₃ (A = K, Rb, Cs; and X = F, Cl, Br) halide perovskite compounds.