Electronic structure and optical properties of the dialkali metal monotelluride compounds: Ab initio study

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#	Paper	IF	Citations
17	Structural, elastic, electronic, magnetic, optical, and thermoelectric properties of the diamond-like quaternary semiconductor CuMn2InSe4. *Journal of Superconductivity and Novel Magnetism*, **2020**, 33, 1091-1102	1.5	25
16	Ab initio study for the structural, electronic, magnetic, optical, and thermoelectric properties of K2OsX6 (X = Cl, Br) compounds. *International Journal of Energy Research*, **2020**, 44, 9035-9049	4.5	18
15	The significance of anti-fluorite Cs2NbI6 via its structural, electronic, magnetic, optical and thermoelectric properties. *International Journal of Energy Research*, **2020**, 44, 10179-10191	4.5	16
14	Influence of the spin-orbit coupling effect on the electronic and thermoelectric properties of Cs2MI6 (M = Zr, Hf) variant perovskites. *Materials Research Bulletin*, **2021**, 134, 111112	5.1	4
13	Study of irradiation temperature effect on change of structural, optical, and strength properties of BeO ceramics when irradiated with Ar8+ and Xe22 heavy ions. *Journal of Materials Science: Materials in Electronics*, **2021**, 32, 10906-10918	2.1	1
12	Structural evolution, lattice dynamics, electronic and thermal properties of VH2 under high pressure. *Solid State Communications*, **2021**, 330, 114287	1.6	4
11	Magnetic, magnetocaloric and thermoelectric investigations of perovskite LaFeO3 compound: First principles and Monte Carlo calculations. *Computational and Theoretical Chemistry*, **2021**, 1204, 113421	2	3
10	Tuning the electronic structure and optical properties of □Te/g-SiC and □Te/MoS2 van der Waals heterostructure. *Materials Chemistry and Physics*, **2021**, 273, 125026	4.4	
9	First-principles calculations to investigate ultra-wide bandgap semiconductor behavior of NaMgF3 fluoro-perovskite with external static isotropic pressure and its impact on optical properties. *Optik*, **2022**, 252, 168532	2.5	2
8	Photocatalytic and tunable optical absorption properties of sandwich-like p-n type LaBO3/KNbO3 (B = Al, Ga) heterostructures. *Physica E: Low-Dimensional Systems and Nanostructures*, **2022**, 139, 115171	3	
7	Ab-initio method to investigate organic halide based double perovskites (CH3NH3)2AgMBr6 (M = Sb, Bi) for opto-electronic applications. *Journal of Materials Research and Technology*, **2022**, 17, 649-657	5.5	1
6	First-principles investigation of structural, optoelectronic, and thermoelectric properties of Cs 2 Tl(As/Sb)I 6. *International Journal of Energy Research*,	4.5	1
5	Ab-initio method to investigate perovskites BiXO3(X = Be, Ca, Mg, Na, K, Li) for spintronics applications. *Solid State Sciences*, **2022**, 126, 106839	3.4	1
4	First-principles investigation of Rb 2 Ag (Ga/In)Br 6 for thermoelectric and photovoltaic applications. *International Journal of Quantum Chemistry*,	2.1	
3	First-principles calculations to investigate the influence of porphyrin substitution on the structural, electronic and optical properties of graphene oxide. *Optik*, **2022**, 257, 168874	2.5	
2	First-principles investigation of Rb2Tl(As/Bi)I6 for green technology. *Chemical Physics Impact*, **2022**, 4, 100071	1.6	1
1	Tuned physical characteristics of PbSe binary compound: a DFT study. **2022**, 18, 649-659		0