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| Title | Semiconductor to metallic transition under induced pressure in Cs2AgBiBr6 double halide perovskite: a theoretical DFT study for photovoltaic and optoelectronic applications | | |
| Author(s) Name | Md. Nurul Islam, Jiban Podder, Tusar Saha, Protima Rani | | |
| Contact Email(s) | [tusar.justphy@gmail.com](mailto:tusar.justphy@gmail.com), [jpodder59@gmail.com](mailto:jpodder59@gmail.com) | | |
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| Abstract |  |
| Inorganic double halide perovskites have a wide range of applications in low-cost photovoltaic and optoelectronic devices. In this manuscript, we have studied their structural, electronic, mechanical and optical properties using density functional theory (DFT) simulations. In this work, hydrostatic pressure is induced from 0 to 50 GPa. Disordered Ag and Bi atoms have a large impact on band gap energy; in this case, the indirect band gap is transferred towards a direct band gap. We have seen that pressure-driven samples have transformed a band energy semiconductor into a metallic one. Under the induced hydrostatic pressure, the covalent bond is transformed into a metallic bond and the bond lengths are reduced. Meanwhile, pressure-induced samples enhance symmetry breaking in [AgBr6]5− and [BiBr6]3− octahedra, which reduces the density of states of the Fermi surface and lowers the total energy. The mechanical behaviors demonstrated that the studied materials are mechanically stable as well as ductile and their ductile nature is enhanced by the driving pressure. The absorption peak is shifted towards the low energy region with increased hydrostatic pressure. The absorptivity and dielectric constant values are also increased with driving pressure. Phase transformed double halide perovskites triggered by outside stimuli produce several outstanding materials properties, giving great scope for a broad range of applications. This type of pristine and disordered double halide perovskite with pressure-driven semiconductor-to-metal phase transition samples may have potential applications in optoelectronic and photovoltaic devices. | |