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| Title | Pressure induced semiconductor to metal phase transition in cubic CsSnBr3 perovskite | | |
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| Abstract |  |
| Phase transitions in metal halide perovskites triggered by external provocations produce significantly different material properties, providing a prodigious opportunity for comprehensive applications. In the present study, the first principles calculation has been performed with the help of density functional theory using the Cambridge Serial Total Energy Package code to investigate the physical properties of lead-free CsSnBr3 metal halides under various hydrostatic pressures. The effect of pressure is determined in the range of 0–28 GPa by the generalized gradient approximation and Becke, three-parameter, Lee–Yang–Parr functions. Subsequently, a significant change is observed in the lattice constant and volume with increasing pressure. The electronic band structure shows a semiconductor to metal phase transition under elevated pressure. The investigation of optical functions shows that the absorption edge of the CsSnBr3 perovskite is shifted remarkably toward the low energy region (red shift) with improved pressure up to 16 GPa. In addition, the absorptivity and dielectric constant also upsurge with the applied hydrostatic pressure. Finally, the mechanical properties reveal the fact that the CsSnBr3 perovskite is mechanically stable and highly ductile; the ductility is increased with increasing pressure. This type of semiconductor to metal phase transition may inspire a wide range of potential applications. | |