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| Abstract |  |
| The antiperovskites based on metal halides have emerged as potential materials for advanced photovoltaic and electronic device applications. But the wide bandgap of non-toxic CsSnCl3 reduces its photovoltaic efficiency. Here, we report the change of electronic structure of CsSnCl3 at different pressure by using GGA-rPBE and GGA-PBEsol functionals and the GW method. We have shown that the prediction of electronic structure transition (semiconducting to metallic state) strongly depends on the exchange-correlation and the GW method gives the most reasonable values of the bandgap under pressure. The pressure increases the electronic density of states close to the Fermi level by pushing the valence electrons upward and thus, reduces the bandgap linearly. Afterward, we have also investigated the influence of pressure on absorption coefficient, and mechanical properties meticulously. Although the pressure shifts the absorption peak to lower photon energies, the absorption coefficient is slightly improved. | |