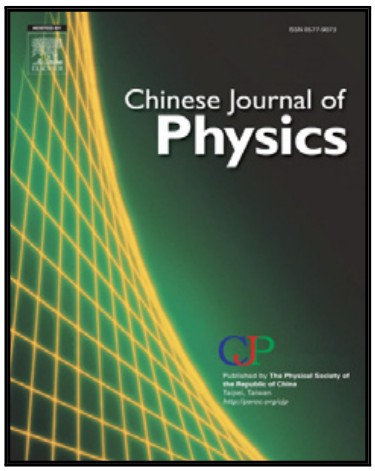

Structural, electronic, optical and elastic properties of the cubic perovskite $PbHfO_3$ through modified Becke-Johnson potential

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Highlights

- The structural, optoelectronic and elastic properties of PbHfO3 were calculated.
- TB-mBJ scheme found to be an efficient approximation for improving the values of the band gap over GGA value.
- The semiconductor character was found by using GGA as well as TB-mBJ approaches.
- PbHfO3 is an attractive and promising material for UV optoelectronic applications.
- Mechanical stability criteria are satisfied for the studied material and classified as ductile in nature.