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Systematic study of elastic, electronic, optical and thermoelectric properties of cubic $BiBO_3$ and $BiAlO_3$ compounds at different pressure by using ab-initio calculations

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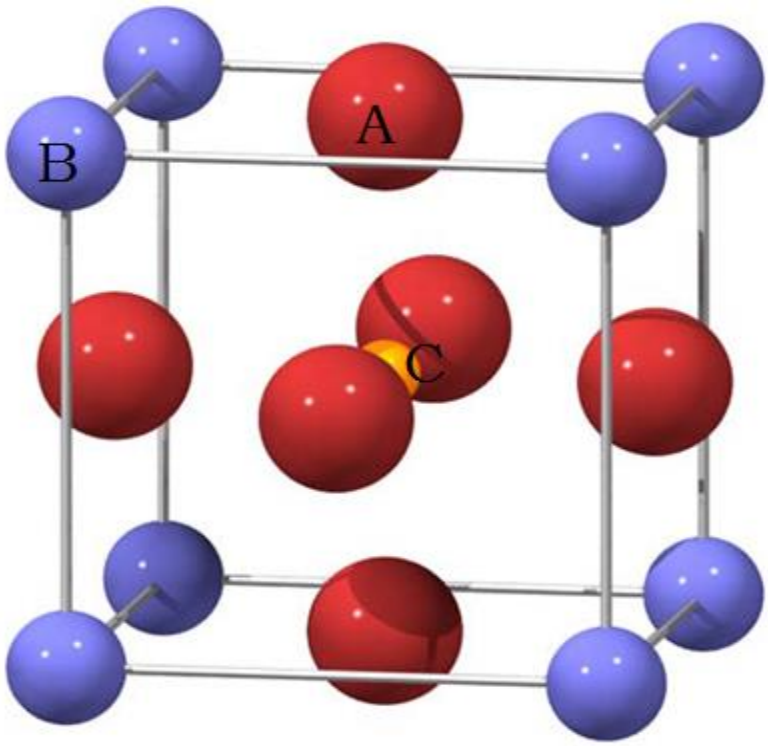
Graphical Abstract



Cubic structures of perovskite oxides ABC_3 (A=Bi, B= B, Al and C=O)

Highlights

- Ab-initio investigation of $BiBO_3$ and $BiAlO_3$ semiconductors under the influence of external pressure is reported.
- Structural and elastic properties are computed for evaluating stability.
- Shift of indirect to direct bandgap is observed at different pressure
- Optical properties have revealed a higher energy shift, as the applied pressure increases proposing potential optoelectronic device applications.