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# High pressure properties of doped ZnO from ab initio calculation

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We performed ab initio calculation based on density functional theory for studying high-pressure properties of doped ZnO. At the beginning, the impurities of Al and Ga atoms into ZnO were investigated up to 10 GPa. The tendency of enthalpy formation under pressure was studied. The high-pressure properties such as lattice parameter, electron density and elastic constant were investigated. It was found that the enthalpy formation of doped ZnO decreases when pressure increasing. The chemical bonds and electron density differences of ZnO unit cells were changed by adding the Al and Ga atoms.

## Summary

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