

## Elastic properties calculation of Hexagonal Gallium Nitride doped with Osmium in the presence of Universal force field

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**Abstract.** Hexagonal GaN is a wide band gap semiconductor of group III/V. It has different applications in the field of laser, storage device, telecommunications etc. In this present work, investigations on the elastic properties of Osmium doped hexagonal GaN is done using the universal force field by DFT method. As the GaN shows the brittle nature, sometimes it is hard to fabricate in a device. So the main motivation of the work to reduce the brittleness of the GaN by doping the malleable and ductile Osmium metal. Osmium metal is corrosion resistive with high melting point. Here various elastic parameters of hexagonal GaN like young's modulus  $Y$ , bulk modulus  $B$ , compressibility  $K$ , Poisson's ratio  $\sigma$ , shear modulus  $G$  calculated on Universal force field using Density functional theory for Os doped GaN at Ga-site as well as N-site. Also processed the elastic stiffness constants  $6 \times 6$  matrix in an elastic tensor analysis (ELATE) software for the 3D illustrations of the various elastics constants.

**Keywords:** GaN, DFT, Osmium, Elastic property, Elastic constants, ELATE, Forcite, Universal Force field