

# On the electronic nature of silicon and germanium based oxynitrides and their related mechanical, optical and vibrational properties as obtained from DFT and DFPT

## Abstract

Electronic structure, bonding and optical properties of the orthorhombic oxynitrides  $\text{Si}_2\text{N}_2\text{O}$  and  $\text{Ge}_2\text{N}_2\text{O}$  are studied using the density function theory as implemented in pseudo-potential plane wave and full-potential (linearized) augmented plane wave plus local orbitals methods. Generalized gradient approximation is employed in order to determine the band gap energy. Indeed, the  $\text{Si}_2\text{N}_2\text{O}$  exhibits a large direct gap whereas  $\text{Ge}_2\text{N}_2\text{O}$  have an indirect one. Bonding is analyzed via the charge densities and Mulliken population, where the role of oxygen is investigated. The analysis of the elastic constants show the mechanical stability of both oxynitrides. Their bulk and shear modulus are slightly smaller than those reported on nitrides semiconductors due to the oxygen presence. The optical properties, namely the dielectric function, optical reflectivity, refractive index and electron energy loss, are reported for radiation up to 30 eV. The phonon dispersion relation, zone-center optical mode frequency, density of phonon states are calculated using the density functional perturbed theory. Thermodynamic properties of  $\text{Si}_2\text{N}_2\text{O}$  and  $\text{Ge}_2\text{N}_2\text{O}$ , such as heat capacity and Debye temperature, are given for reference. Our study suggests that  $\text{Si}_2\text{N}_2\text{O}$  and  $\text{Ge}_2\text{N}_2\text{O}$  could be a promising potential materials for applications in the microelectronics and optoelectronics areas of research.