

COCEMASOV, A., BRINZARI, V., NIKA, D. Energetic, structural and electronic features of Sn-, Ga-, O-based defect complexes in cubic In₂O₃. In: Journal of Physics: Condensed Matter. 2021, Vol. 32, Nr. 22, 225703. ISSN 0953-8984.

Defect energy formation, lattice distortions and electronic structure of cubic In₂O₃ with Sn, Ga and O impurities were theoretically investigated using density functional theory. Different types of point defects, consisting of 1–4 atoms of Sn, Ga and O in both substitutional and interstitial (structural vacancy) positions, were examined. It was demonstrated, that formation of substitutional Ga and Sn defects are spontaneous, while formation of interstitial defects requires an activation energy. The donor-like behavior of interstitial Ga defects with splitting of conduction band into two subbands with light and heavy electrons, respectively, was revealed. Contrarily, interstitial O defects demonstrate acceptor-like behavior with the formation of acceptor levels or subbands inside the band gap. The obtained results are important for an accurate description of transport phenomena in In₂O₃ with substitutional and interstitial defects.