Structural and Electronic Properties of Ge Polytypic Junctions from an A*b-initio* Perspective

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The thermodynamic ground-state bulk crystalline Ge at ambient conditions takes a cubic-diamond (*c*-Ge) structure. Nevertheless, the existence of hexagonal-lonsdaleite (*h*-Ge) phase has been recently observed in Ge nanowires in the form of crystal imperfections (e.g., stacking-faults) [1] or as a consequence of a strain induced phase transformation [2]. Interestingly, these nanowires present a stable polytypic mixture of *c*-Ge and *h*-Ge allotropes. As a consequence, the comprehension of their fundamental properties has emerged as an important research subject because of their enormous potential for technological applications [3-6]. Here, we employ accurate hybrid Density Functional Theory (hybrid-DFT) methods to calculate the structural and electronic properties of *h*-Ge and *c*-Ge/*h*-Ge interfaces [7]. First, we present a comparison of *h*-Ge with respect to *c*-Ge that reveals three major differences: **i)** a reduction in the band gap value, **ii)** a transition from an indirect-gap to a direct-gap semiconductor (as depicted in Figure 1) and **iii)** a red-shift of the optical spectra. Second, the study of the polytypic junctions, carried out by taking into account the presence of *h*-Ge segments in a pure *c*-Ge system, shows that **i)** the structural discontinuity at the interface causes only minor atomic rearrangements, **ii)** the *c*-Ge/*h*-Ge interface induces a type-I band offset where the valence and the conduction band edges are both located at the centre of Brillouin zone in the *h*-Ge region [7]. Our findings indicate that fabricating Ge polytype junctions is an alternative route to band structure engineering which could improve the functionalities of novel electronic and optoelectronic devices.

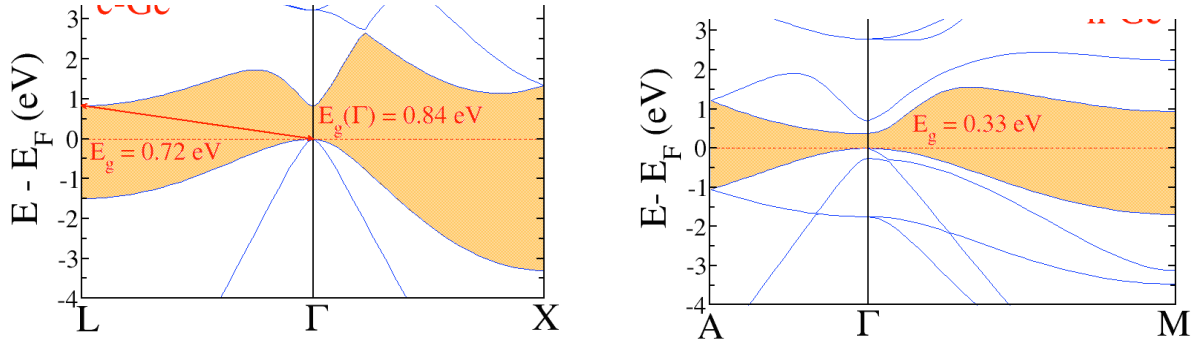

Figure 1. Band diagram of crystalline *c*-Ge (left panel) and *h*-Ge (right panel).

Keywords: Ge heterostructure, Band offsets, Hybrid functional DFT, Hexagonal-lonsdaleite

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