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Electronic structure of (Si)GeSn and its tuning via incorporation of carbon

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Abstract: The electronic band structure, and in particular the band gap directness, of binary and ternary SiGeSn alloys are first reviewed, and different aspects of their optoelectronic and microelectronic applications discussed, and the computational analysis is then extended to the dilute carbon-containing alloys.

With the advances in group-IV photonics (and also electronics) a reliable knowledge of the electronic band structure of CSiGeSn alloys, including their ternary and binary subsets, is increasingly important for the design considerations of various components based on them [1], with the eventual target being the integration of group-IV alloy based (opto)electronic components on silicon substrate, with all the benefits coming from mature and cost-effective fabrication. The directness of the band-gap is very important for optoelectronic devices (primarily lasers [2], but also LEDs, photodetectors and modulators), very much improving the device performance. However, directness may also be important in purely electronic devices, e.g. delivering a higher electron mobility. Except by the composition, the values of the direct and indirect gaps can be controlled by strain, and if this is to be exploited a good knowledge of the deformation potentials in these alloys is also necessary.

Some of the group-IV alloys have been studied in considerable detail, both experimentally and theoretically. On the theoretical side, methods of different complexity have been used, like ab-initio methods, self-consistent pseudopotentials, empirical pseudopotentials, etc., e.g. [3-6]. We first review recent studies of the band structure of SiGeSn, and discuss the potential of these alloys for optoelectronic applications, and then also consider carbon-containing alloys, where different predictions of the effects of incorporation of carbon on the alloy band gaps have been made, e.g. [5-7].

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