FIRST-PRINCIPLES CALCULATION of ALLOY SCATTERING in $Ga_xIn_{1-x}As$ using QUANTUM ESPRESSO CODE

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ABSTRACT - In materials and device design, III-V semiconductor alloys (e.g. GaInAs) are widely used in high-mobility applications. Many factors in the construction of these devices affect the transport properties - e.g. alloy disorder, inter-valley or intra-valley phonon scattering, interface roughness. However, experimental measurements have been unable to unambiguously separate these contributions. As a result, alloy scattering in these materials is not quantitatively well understood. Recently, ab intio electronic structure methods [1-3] have been developed in our research group, which provided the first quantitative description of alloy scattering in bulk SiGe alloys from first principles. We aim to adapt these techniques to study the corresponding question in III-V alloys. The goal of this project is to utilise the Lanzcos-GW (GWL) computational technique [4,5], recently incorporated in the Quantum ESPRESSO electronic structure code to compute the quasi-particle energies needed to calculate alloy scattering in III-V semiconductors. This project aims to build on work that has already been undertaken in a previous Class C project on the ICHEC Stokes cluster, a HPC-Europa2 project on CINECA machines, and is part of the research work supported under a current SFI Principal Investigator (PI) Programme.

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