Internship

Electronic structure of bulk semiconductors, alloys and heterostructures based on InSb including strains .

The electronic structure of materials is the key point to understand their behavior. Its calculation requires successive approximations because computing the full Hamiltonian of the "complete" crystal is out of range, even for most efficient computers.

The electronic structure gives access to various parameters such as: dielectric function, piezoelectric tensor, inter-atomic force constant for the dispersion of phonons, and it appears to be crucial in various tools devoted to transport modeling (Monte Carlo, NEGF…).

Several approaches for band structure calculations are available, such as the ab-initio method and semi-empirical ones. The later need adjustment parameters and provide satisfactory results (up to 5-6 eV from both sides of the forbidden bandgap). Most of the time, it is enough, but these semi empirical models are not always easy to obtain due to the lack of measurement results. Then Ab-initio calculations are mandatory.

We propose an internship based largely on the density functional theory (DFT) to access to the electronic structure. For this, the candidate will use either the Quantum Espresso or Abinit softwares, to calculate first the electronic structure of a little known bulk materials such as InSb or ternary alloys as $In_{1-x}Al_xSb$ useful for the realization of high-performance IR photo-detectors. The very strong spin-orbit coupling of InSb makes a little more difficult the calculations of the electronic structure. Then, the strain effects in InSb and in $In_{1-x}Al_xSb$ alloys will be evaluated. Thirdly, the heterojunction $InSb/In_{1-x}Al_xSb$ will be calculated.

The results using various functionals of exchange and correlation (GGA and hybrids) will be confronted to G_0W_0 when it should be relevant. The advantage of the GGA functional or hybrids is the calculation speed but in this case the energy gap is, most of the time, underestimated.

The band structures calculated in the frame of the DFT method will allow to improve the calculation performed by k.p multiband method and by empirical pseudopotentials approach (EPM). These last tools are well suitable when millions of calculations have to be generated as it is the case for Monte-Carlo simulators because Hamiltonian' sizes of k.p and EPM are far smaller than within the DFT approach.

This work may give rise to a PhD continuation.

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