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The Electronic Structure of Heterostructured and Superlatticed Si/Ge Nanowires: A Maximally-Localised Wannier Function Approach
MATTHEW SHELLEY, ARASH MOSTOFI, The Thomas Young Centre, Imperial College, London — In recent years, Si/Ge nanowires have generated much interest within condensed matter and electrical engineering communities due to the variety of tunable properties that they exhibit. Heterostructured or superlatticed Si/Ge nanowires have been identified as potential candidates for such thermoelectric applications[1] and a detailed knowledge and understanding of their electronic structure would help exploit or maximise this effect. Modelling such systems is a serious challenge for traditional electronic structure methods, such as density functional theory (DFT). The study of systems that are non-periodic, or have very large periodic repeat units, is prohibitive with the traditional plane-wave (PW) formalism of DFT. We have therefore developed a method which combines the accuracy of large-scale PW-DFT calculations with the transferability of a compact basis of maximally-localised Wannier functions (MLWFs). Moving to a MLWF basis allows the Hamiltonians of fragments of a system to be combined to form model Hamiltonians of large disordered systems. We present results on heterostructured and superlatticed Si/Ge nanowires in the ballistic regime with a view to discuss their thermoelectric merit.

[1]Li *et al* Appl. Phys. Lett. **83** 3186 (2003)

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