Multiscale approach to treating random alloy effects in III-N nanostructures

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The importance of nitride-based materials was recognized with the award of the 2014 Nobel Prize “for the invention of efficient blue LEDs”. Surprisingly, there remain many challenges: not just to further enhance the efficiency of blue LEDs but also to develop LEDs that emit efficiently across a wider spectral range. However, electronic properties of III-N heterostructures are dominated by large internal built-in polarization fields, as well as by the impact of random alloy effects. A multiscale approach is required to describe key details of the electronic structure of III-N materials, and its consequences for devices. In a first step, we have performed hybrid functional DFT calculations to extract key material parameters, such as piezoelectric polarization coefficients using the Berry-Phase technique. Secondly, we have developed a local polarization theory, showing excellent agreement with Berry-Phase results. Thirdly, a tight-binding model has been developed, by fitting and benchmarking against DFT data. This model can now treat $10^5$ atoms, allowing for an accurate description of random alloy effects. We overview the developed models and provide critical insight into the nanoscale electronic properties of such alloys. We provide also key parameters required for continuum-based device models.