Atomistic simulations with experimentally estimated atomic positions in a SiGe quantum well

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Current miniaturization trends and emerging quantum technologies call for an almost atomistic control of device fabrication, to the point where "every atom counts" towards the final device properties. The properties of semiconductor spin qubits, for example, depend sensitively on local strains [1] and compositional disorder, notably at interfaces [2,3]. It would thus be desirable to use experimentally determined atomic positions as inputs to atomistic simulations, to compute and understand the properties of systems "as grown". In this work [4], we present proof of concept calculations in this direction, taking advantage of a recently introduced AI-assisted microscopy workflow, which is able to estimate atomic positions from experimental micrographs [4]. We base our calculations on such estimated 3D atomic models for the quantum well of a silicium-germanium planar heterostructure semiconductor hole spin qubit [5] (fig. 1), and compute variations of the local vibrational and electronic densities of states along the growth direction, using respectively the Keating model [6] and a tight-binding model [7] along with linear scaling methods [8,9], which allow for the simulation of multi-million atoms systems. We further emphasize the interest of computational methods to assess the quality of 3D atomic models by showcasing an example where they reveal the impact of microscopy acquisition errors that were initially undetected by the naked eye.

References

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Figures

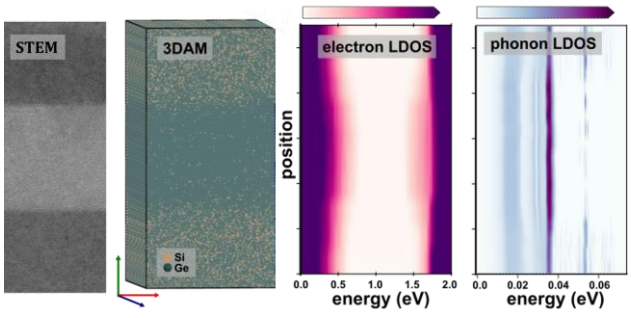

Figure 1: left to right: illustrative examples of experimental STEM image and estimated 3D atomic model (3DAM) of a SiGe quantum well with computed vibrational and electronic LDOS (position alignment illustrative - see [4] for details).