Atomistic Simulation of Ge/SiGe Interfaces for Quantum Technology Devices

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The accurate modeling of Ge/SiGe nanostructured devices remains a fundamental challenge in the design and optimization of quantum technologies, particularly for hole-based quantum wells. The unknown atomic arrangement and disorder at the Ge/SiGe interface, combined with the complex strain distribution, significantly affects the potential landscape and hinders theoretical predictions beyond gross approximations on the potential experienced by the hole. Traditional atomistic simulations struggle to capture these effects, either due to their limited scalability (ab initio) or the impossibility to capture complex chemical environments at the interface (empirical potentials). In this contribution, we overcome these challenges by leveraging universal machine learning (ML) interatomic potentials, fine-tuned on Ge/Si/SiGe databases with different stoichiometries and disorders. Our approach enables efficient and accurate modeling of large-scale nanostructured systems and offers a critical step toward reliable simulations of the electronic properties of quantum wells and Ge/SiGe heterostructures by improving the description of atomic disorder and strain effects, thereby enhancing qubit design and performance optimization.

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