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Atomistic Configuration Interaction Simulation Tool for Semiconductor Based Quantum Computing Devices

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ABSTRACT

Solid-state devices are promising candidates for quantum computing applications due to obvious advantages in compatibility with semiconductor fabrication technologies and the extremely long coherent times of electron and nuclear spins in these devices. In such devices, electron interactions are crucial for single and two qubit gate operations. Thus it is essential to evaluate these electron-electron interactions accurately for precise qubit control. It is shown that Atomistic Configuration Interaction can be used to accurately determine electron-electron interactions in realistic semiconductor quantum computing devices. In this work, an online simulation tool on Atomistic Configuration Interaction has been implemented and published on nanoHUB.org, a web interface for computational nanotechnology research, education and collaboration. The tool runs on simulation engines (1) NEMO to simulate realistic device structures on an atomic scale using tight-binding to obtain single electron wave functions and; (2) Configuration Interaction to solve the few-electron Schrodinger equation in the Slater Determinant basis of the selected single electron wave functions. The GUI of the tool supports a large set of input options to specify the parameters for electrostatically and Coulomb defined single-electron quantum dots. Atomistic Configuration Interaction simulations are computationally intensive and can be submitted on RCAC supercomputing clusters via the tool. The results from the tool have been benchmarked against data from literature for double quantum dots loaded with two electrons, to study electron exchange interactions. The good qualitative agreement gives us confidence in the simulation tool and has been provided as example simulations in the tool. The user-friendly Atomistic Configuration Interaction tool made available through nanoHUB is ready to be employed by researchers and students for studying few-electron systems in semiconductor devices.

KEYWORDS

Quantum Computing, Semiconductor, Simulation