

Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics

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Almost all of the proposed solid-state qubit devices and circuits rely on a nano-scale semiconductor implementation. Experimental efforts are limited by physical nano-scale characterization methods in an overwhelmingly vast design space (material systems, doping levels, gating, free charges). At present, all studies in the literature that model heterostructures comprising a quantum computing device make simplistic physical assumptions. For example, single band jellium models, which take into account only band edges and effective masses, are usually employed to describe the electronic structure. It has been shown that such an assumption, while appropriate for a rough device concept, is insufficient for actual device designs and characterizations. Only realistic models which include bandstructure, carrier distribution throughout the device (including contacts) and de-coherence mechanisms will enable the appropriate treatment of the coupled quantum systems and, ultimately, circuits. We plan to fill this void by the development of an atomistic nanoelectronic device simulation tool which will aid the design of spintronic qubit devices and circuits and their parameterization in higher level qubit circuit models. We have recently developed a nanoelectronic modeling tool entitled NEMO 3-D prototype that enables the atomistic simulation of electronic structures that contain several million atoms. NEMO 3-D is based on the previous development of NEMO 1-D at Texas Instruments and JPL, which is the state-of-the-art heterostructure transport simulation tool. This presentation will outline the status of the NEMO 1-D and 3-D simulators with respect to electronic structure and transport simulations in nano-scaled devices such as quantum dots and resonant tunneling diodes. Our plans to expand these tools to enable the simulation of spintronic transport will be outlined.

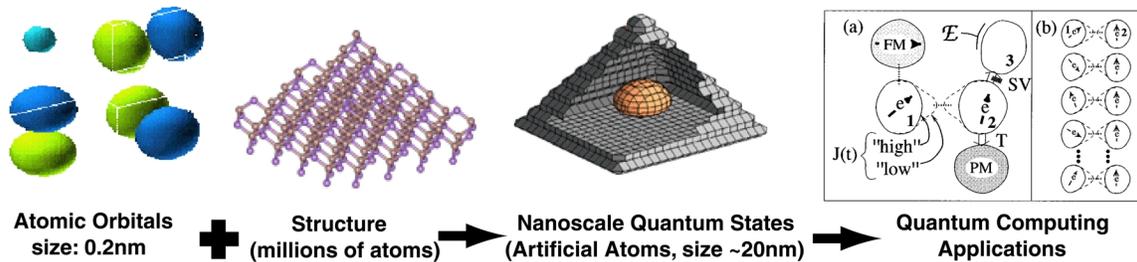


Figure 1. Our approach to Nanoelectronic modeling: link the actual representation of electronic orbitals in the sub-nanometer length scale to nanometer scale quantum phenomena and map these phenomena and their interactions to quantum computing applications. The very right panel is taken from the quantum dot based proposal by Loss and DiVincenzo (Loss, D. and D.P. DiVincenzo, Phys. Rev. A, 1998, **57**, p. 120.).