JPUR
JOURNAL OF PURDUE
UNDERGRADUATE RESEARCH

ENGINEERING/TECHNOLOGY

Incorporating Magnetic Fields into NEMO5

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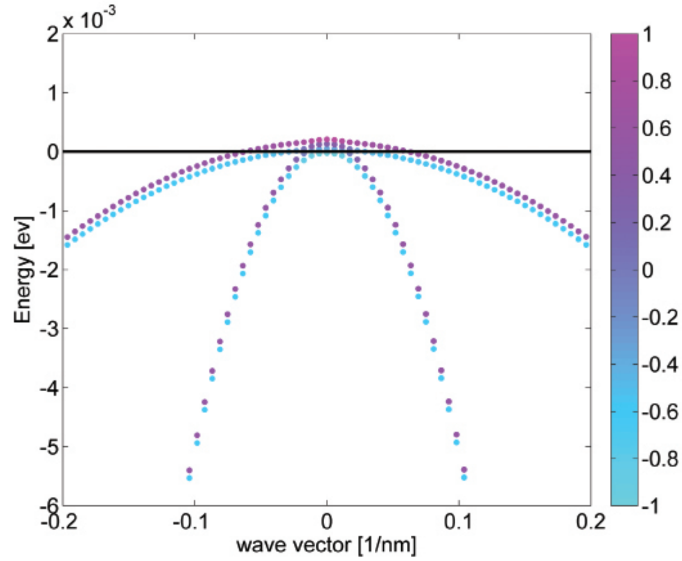
The miniaturization of semiconductor device technology corresponds directly to faster, more powerful, and smaller computing systems. However, designing, prototyping, and constructing effective components for such devices becomes enormously complex and expensive and cannot be performed experimentally alone. In general, modeling and simulation approaches are used to help create new device generations. However, we are now reaching device sizes that are defined by just a few atoms, and almost all existing modeling tools represent materials in a continuum approach, without considering atoms. The nanoelectronic modeling (NEMO) tool suite models devices explicitly atomistically (completely quantum mechanically). The exploration of the device physics often includes the use of magnetic fields to probe the electronic structure in the device. In previous versions of NEMO, magnetic fields were used; therefore, this research involved writing code to apply constant and uniform magnetic fields to the current version of NEMO (NEMO5), under gauge invariant constraints. The method used has two parts: the Peierls phase and Zeeman splitting. First, the Peierls phase weighs the empirical tight binding offsite Hamiltonian matrix elements. Then, Zeeman splitting is done by augmenting the Hamiltonian with the addition of a Zeeman factor. These factors directly change the Hamiltonian, allowing for the study of the Hamiltonians, band structures, and eigenvalues of the GaAs sp3d5s* structures and the Si sp3d5s* structures (both with and without spin orbital interactions). The work done in this research will be used to help validate NEMO5 and potentially to simulate spintronic devices. Future work on this project will be mainly on the Peierls phase code validation and optimization.

Research advisor Gerhard Klimeck writes, "Travis worked on an expansion of a sophisticated nanoelectronic modeling tool (NEMO5). NEMO5 is used to study nanoscale transistors and research devices such as single-atom transistors. It is often critical to examine such devices subject to an external magnetic field. Travis integrated a homogeneous magnetic field into NEMO5."



Spin split band structure of GaAs sp3d5s*-SO caused by an implemented magnetic field generated by a NEMO5 simulation.

Sheperd, T. (2013). Incorporating magnetic fields into NEMO5. *Journal of Purdue Undergraduate Research*, 3, 88-89. http://dx.doi.org/10.5703/1288284315179