LEADING FUTURE ELECTRONICS INTO THE NANO REGIME USING QUANTUM ATOMIC SIMULATIONS IN NEMO5

Research Challenge
The semiconductor industry influences approximately 10% of the world GDP, either directly or through electronic systems. Continuous speed and power consumption improvements must be made to the transistor technology for the stability and growth of the industry. Further improvements in shrinking dimensions will come only through the detailed study of device designs, materials, and of quantum effects such as tunneling, state quantization, and atomistic disorder. This project addresses these issues and others on a variety of semiconductor devices through simulation.

Methods & Codes
The team uses NEMO5, available at nanoHUB.org, to perform multi-physics atomistic quantum simulations. Topics of study include quantum transport simulations for transistors, the current mechanism of tunneling field-effect transistors, tunneling transistors, quantum computing devices such as quantum dots, multi-scale quantum transport simulations for certain LEDs, and others.

Results & Impact
- Nitride device simulations have been used to suggest improvements to the multi-quantum-well nitride-based LED.
- Simulations have led to the proposal of a new alloy engineered nitride tunneling field-effect transistor as a novel low-power transistor design.
- A new computational method for modeling incoherent scattering phenomena in electron transport, which provides shorter times-to-solution and smaller memory footprints, has been added to NEMO5.

Why Blue Waters
Quantum transport fundamentally deals with non-equilibrium phenomena that involve multi-particle interactions. Such simulations are conceptually and computationally more demanding that traditional ab-initio materials simulations. Blue Waters was used for running such simulations on up to 16,384 cores per simulation. In many cases the work could not be accomplished in a reasonable amount of time without Blue Waters, and for the larger simulations the work could not be accomplished on other available systems.

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