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

Research Challenge
The United States has always been a world leader in the semiconductor industry with 40% of the worldwide semiconductor device-related patents originating here. The U.S. holds one-third of the global semiconductor device market, which is worth over $300 billion per year. Simultaneously, a relentless reduction in semiconductor size is occurring, with devices expected to be about 5 nanometers long in their critical active region within 10 years. Further improvements in shrinking dimensions can come only through detailed study of device designs, materials, and quantum effects. Complex, fundamental questions remain. NEMO5 was developed by the Institute for NanoElectronic Modeling (iNEMO) at Purdue University to address these fundamental issues. NEMO5 enables basic engineering, physics, and material research, and is used by leading semiconductor firms to design future devices.

Methods & Codes
iNEMO’s research on Blue Waters encompasses multiphysics atomistic quantum simulations implemented in NEMO5. The needed physics vary from one device to another, but all can be simulated inside NEMO5. Some examples are:

• Quantum transport simulations (for transistors) using an approach employing semi empirical tight-binding methods.
• Multiscale quantum transport modeling that represent regions of high- and low-electron densities
• Atomic basis sets mapped from established, fundamental methods, and resulting in models that can represent realistically extended devices

Why Blue Waters
Quantum transport simulations are very computationally expensive and demanding of memory due to the high degree of complexity of the equations used. 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. Blue Waters’ staff provide exemplary support and user outreach to guide system usage, help with issues as they arise, and assist with code performance and scaling.

Results & Impact
Aggressive semiconductor downscaling into a countable number of atoms in the critical dimensions makes atomistic simulations necessary pathfinders in the quantum regime. NEMO5 is designed to comprehend the critical multiscale, multiphysics phenomena for nanoscale technology through efficient computational approaches and enables quantitative study of new generations of nanoelectronic devices even beyond transistors.