Research Challenge
This project focuses on high-performance calculations for materials and devices, and on development of petascale methods for such simulations. The research challenges are the investigation of sensor configurations for detection of biologically important molecules, the analysis of high-performance dielectric materials that store and release energy electrostatically through polarization and depolarization, and the pursuit of atomically precise and bottom-up fabrication of graphene-based electronics.

Methods & Codes
The quantum transport and large-scale electronic structure calculations rely on the use of the RMG code developed by the team. Polymer simulations employ the LAMMPS code. Calculations that include van der Waals interactions use the PWSCF code.

Results & Impacts
The studied glucose sensor configuration and mechanism opened the path to the design of other nanotube sensors. The project found that blending a poly(arylene ether urea) (PEEU, $K = 4.7$) and an aromatic polythiourea (ArPTU, $K = 4.4$) leads to a compound that exhibits a very high dielectric constant, $K = 7.5$, while maintaining low dielectric loss (< 1%). The team established how the bottom-up synthesis of a graphene nanoribbon can be controlled by charge injections from a scanning microscope (STM) tip.

Why Blue Waters
The conducted applications require very large compute and high-speed interconnect resources that are available on Blue Waters. Each project requires performing many runs to explore the various scientific issues, with a substantial amount of analysis between the runs. High availability and quick turnaround that Blue Waters provide are essential for success of the project.