BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Allocation: Illinois/550 Knh

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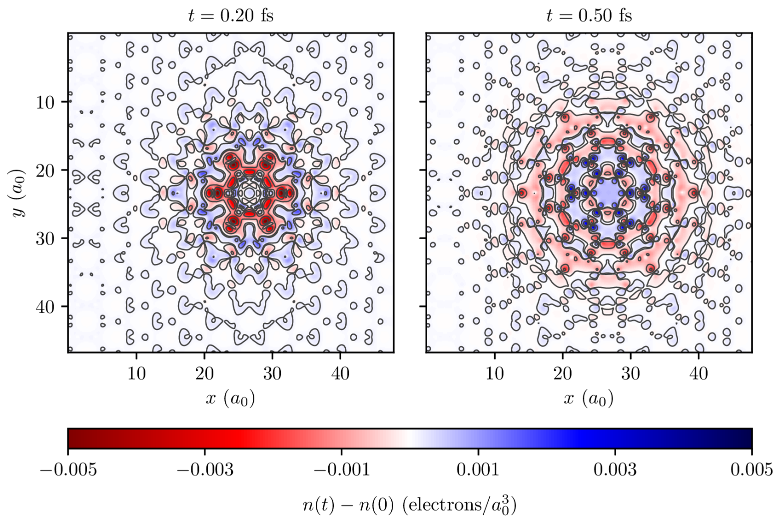
Physics & Engineering

ELECTRON DYNAMICS IN ION-IRRADIATED GRAPHENE



Visualization of local charge in graphene 0.2 and 0.5 femtoseconds after a proton impacts the material. Blue indicates negative charge while red indicates positive charge.

Research Challenge

To understand extremely fast quantum-mechanical processes involving electrons in atomically thin carbon sheets (graphene), which is important for developing radiation-resistant materials and advancing imaging and fabrication techniques for next-generation electronic materials.

Methods & Codes

The team uses Qbox/Qb@ll, their parallel implementation of time-dependent density functional theory. This treats nuclei as classical point charges interacting electrostatically with electrons. Electrons are treated quantum-mechanically; their quantum orbitals are governed by the time-dependent Kohn–Sham equations and are related to the time-dependent electron density. This approach provides accurate information about charge and energy dynamics at time and length scales inaccessible to experiment.

Why Blue Waters

Blue Waters provided the capability to evolve thousands of electrons over thousands of time steps in a large simulation cell. These aspects, which are necessary for accurate predictions, make the simulations computationally expensive; the team was able to compute detailed information about more than 20 setups with different graphene thicknesses and projectile species, charges, velocities, and trajectories.

Results & Impact

The team evaluated the suitability of certain parameter combinations for imaging two-dimensional materials and found nearly no change in electron emission for 25–80 keV protons impacting graphene. These findings suggest that proton energies of 25 keV and below are optimal for imaging applications, where high electron emission coupled with low damage to the material are desirable. Such findings inform cutting edge tools for high-resolution microscopy and structure modification of graphene and other two-dimensional materials, whose properties are often sensitive to defects.