Enhancing detection with DFT and MBPT: Charge mobility in a Germanium dark matter detector

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A current interest in experimental physics is to build detectors capable of detecting interactions that deposit extremely small energies - down to the 10-eV scale.[1] The dark-matter community, the neutrino-detection community, and the nuclear-monitoring community all gain dramatic increases in signal sensitivity by pushing detector thresholds lower. Many such experiments use a crystalline detector (Si, Ge, NaI_2), detecting a potential dark matter "kick" to a nucleus within by sensing charge, phonons, or light created by the energetic nucleus. But at such low energies (from the perspective of measuring a single ionizing interaction), understanding electron mobility becomes increasingly important. Therefore, a computational approach is undertaken to study electron behavior within the detector.

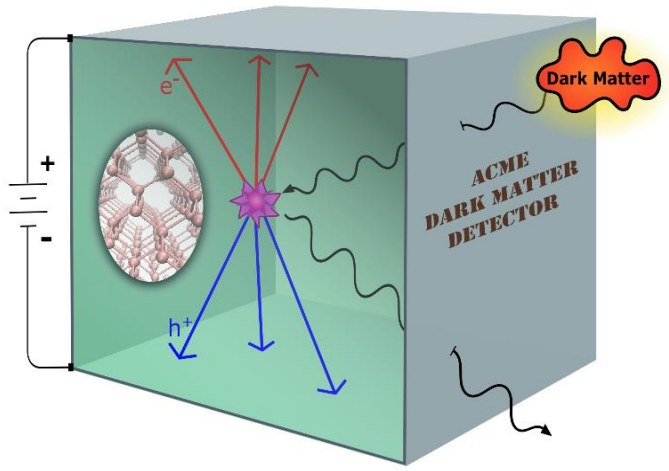

Figure 1 A hypothesized dark-matter interaction. A dark matter particle transfers energy to the crystal, which creates free charge carriers in the detector material. An applied electric field drifts the electrons and holes through the material, allowing their detection. For very low-energy interactions, an accurate understanding of charge mobility is critical to interpreting signals in the detector correctly.

Atomic-level simulations (using the Vienna *ab Initio* Simulation Package with PAW potentials, PBE functional, and a plane-wave basis set) will help answer some of the questions encountered by experimental physicists seeking to measure - and correctly interpret - energy depositions that approach the lattice binding energy. To simulate bulk material, two periodic unit cells of Germanium with differing volumes were created (1400 and 5000 $Å^3$). Prior to investigations of electron-nuclear and nuclear-nuclear interactions, a systematic exploration of the electronic properties and dynamics is planned. To this end, density functional theory (DFT) combined with density matrix equations[2] of motion are used to study the effect of lattice changes (i.e. impurities, vacancies) on charge mobility.

Many of these low-threshold experiments measure ionization; members of the Cryogenic Dark Matter Search (SuperCDMS) have studied the charge mobility as a function of the temperature and voltage applied to Ge detectors. Modeling electron and hole relaxation rates with DFT and density matrix methods allows for direct comparison of simulated calculations with experimental data. Additionally, Simultaneous generation of multiple electron-hole pairs is estimated based on anybody perturbation theory (MBPT).[3] Preliminary calculations indicate that the stability of the crystal lattice is vulnerable to excitation, causing vibrational fluctuations which may affect the function of the detector. In addition, the dynamics of electrons are monitored for simulated energy deposition events.

1. Agnese, R.; Anderson, A., *et al.*, *arXiv preprint arXiv:1610.00006* **2016**.
2. Kilin, D. S.; Micha, D. A., *J. Phys. Chem. Lett.* **2010,** *1* (7), 1073-1077.
3. Kryjevski, A.; Kilin, D., *Mol. Phys.* **2016,** *114* (3-4), 365-379.