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First principles calculation of bulk semiconductor mobilities for radiation detection application VINCENZO LORDI, DANIEL ABERG, ANDREW WILLIAMSON, Lawrence Livermore Lab — The development of high energy resolution, room temperature semiconductor radiation detectors requires the development of materials with both an increased carrier mobility-lifetime product ($\mu\tau$) and a band gap in the 1.6-2.5 eV range. An adequate $\mu\tau$ is required for efficient collection of generated carriers from large devices, maximizing S/N ratio and resolution. We use density functional theory to study the microscopic mechanisms of mobility degradation from point defects and to calculate the intrinsic limits of mobility for a given bulk material. Scattering rates obtained from the Born approximation allow us to calculate the contributions of different point defects on mobility degradation, within Boltzmann transport theory. Both native defects and impurities were considered. Formation energies for the various defects were calculated to determine their equilibrium concentrations. Combined with calculations of the defect chemical potentials, we make predictions on the feasibility of improving mobility by thermal annealing to remove the most detrimental defects. This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

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