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Ab-Initio investigation of defects in GaTe[1] CEDRIC ROCHA LEAO, VINCENZO LORDI, Lawrence Livermore National Lab — Materials that are good candidates for room-temperature radiation detectors should ideally possess several characteristics that are sometimes contradictory. A high carrier mobility-lifetime product is required to maximize the collection of radiation generated charge, but a relatively large bandgap is desired to minimize thermal noise. High resistivity is usually also desired, to reduce background current which degrades the detection resolution. Furthermore, a high average atomic number increases absorption of high energy radiation. GaTe is attracting recent attention for the potential to satisfy many of these criteria, but its properties are still poorly understood. Like other III-VI compounds, GaTe is a layered material, but its unusual anisotropy in the atomic planes results in rather unique mechanical and electronic properties. In this talk, we discuss ab-initio calculations of the transport properties of GaTe with respect to its application to radiation detectors. Guided by very recent experimental results, we analyze the occurrence of native defects in this materials and possible compensating extrinsic defects, and their effects on the transport properties.

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