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Ab-initio guided optimization of layered semiconductors (GaTe,GaSe) for Radiation Detection Applications[1] CEDRIC ROCHA LEAO, VINCENZO LORDI, Lawrence Livermore National Lab — The performance of high resolution semiconductor based radiation detectors at room temperature is hindered by intrinsic defects and accidental impurities. Experimental efforts to improve the properties of such materials are both time consuming and expensive, since they rely to a large extent on trial and error. In this talk, we show how a fully ab-initio approach allows ranking the most detrimental defects in a crystal in terms of carrier recombination and charge transport. The method was applied to gallium telluride and gallium selenide, both moderate gap layered semiconductors. Based on our results, we can tailor experimental processes to grow these semiconductors with optimal properties. This can be achieved by tuning the growth conditions to avoid the most harmful defects or by compensating them through the introduction of dopants that counteract their detrimental electronic behavior without adding significant scattering to propagating wavepackets in the material.

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