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Information-based screens for deep traps in semiconducting materials[1] KIM FERRIS, KUNAL SHAH, Pacific Northwest National Laboratory, DUMONT JONES, Proximate Technologies, LLC. — The key to a successful materials search is the ability to suggest promising materials and a priori eliminate unfruitful inquiry. For semiconducting radiation detection materials, performance is characterized by several key properties; band gap, density, electron mobility, and carrier lifetime. The material's proclivity to form defects is critical, as even simple antisite and vacancy defects can be sufficiently deep to affect effective carrier lifetime and mobility. We have developed a new model for defect formation proclivity, leveraging prior defect models (van Vechten and Feichter) and our information-based work. Our approach is based upon classification of materials chemistry and properties consistent with high concentrations of particular defects (e.g. antisites and vacancies). One issue is that nearly any charged local defect can potentially form a deep trap, so the screen must cover different defect types. Second, the screening model for new materials cannot rely on generally unknown factors such as 3D crystal geometry. The resulting model is intended to provide design guidance on expected defect behavior for candidate detection materials for which there is little or no prior information.

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