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Materials Discovery: Informatic Strategies for Semiconducting Radiation Detection Materials KIM FERRIS, Pacific Northwest National Laboratory, DUMONT JONES, Proximate Technologies, LLC, BRIAN SCHULTZ, International Technology Center — Inorganic semiconducting materials used in gamma radiation detection applications are typically binary and ternary inorganic crystals. Performance metrics for these materials include band gap, relating to carrier concentration and thermal background current; density, relating to stopping power; and electron mobility, which limits electron transport and is typically the dominant information carrier. In this paper, we describe an information-based approach to the identification of new radiation detection materials, using the specific case of the II-VI semiconductors. Even for simple binary systems, the sheer number of potential materials considering the presence of crystal system polymorphs and higher order compositions is daunting. The key to a successful materials search is the ability to suggest promising materials and a priori eliminate unfruitful inquiry. The success of an informatics-based design program depends on the relation of materials-level properties to atomic-scale properties that change rationally with structure, and the ability to extract rules which define these mappings. A brief example of a property-level screen will be given to illustrate the materials development process. The authors gratefully acknowledge financial support from U.S. Department of Homeland Security under Contract No. HSHQDC-08-X-00872.

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