

Abstract Submitted
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First-principles study of defects in TlBr¹ MAO-HUA DU, Oak Ridge National Laboratory — TlBr is a promising radiation detection material due to its high gamma-ray stopping efficiency, high resistivity (that reduces dark current and noise), large enough band gap of 2.68 eV (suitable for room temperature applications), and long electron carrier lifetime (for efficient collection of the radiation-generated carriers). The defect properties obtained from density functional calculations will be presented to discuss their roles in carrier trapping and recombination (which affects the carrier lifetime) and carrier compensation (which affects the resistivity).

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Mao-Hua Du
Oak Ridge National Laboratory

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