

Abstract Submitted
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Diffusion of point defects in CdTe¹ JOHN JAFFE, CHARLES HENAGER, Pacific Northwest National Lab — We have investigated the mobility of isolated native point defects in CdTe by first-principles calculations. Cd vacancies and interstitials, Te interstitials and Te-on-Cd antisites were considered. Diffusion barriers were found by the NEB (nudged-elastic-band) technique within the PAW-LDA method as implemented in the VASP code. Diffusion constants are estimated, and some implications for the growth of radiation detector material are suggested, especially in regard to the formation of Te precipitates. Comparisons to experimental and earlier theoretical studies are also provided.

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John Jaffe
Pacific Northwest National Lab

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