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Diffusion of Interstitial Defects in CdTe[1] SU-HUAI WEI, JI-HUI YANG, JIE MA, JOONGOO KANG, National Renewable Energy Laboratory —
CdTe is one of the most promising candidates for thin-film photovoltaic applications and it is well known that Cu and Cl diffusions play critical roles in improving the CdTe solar cell efficiency. However, the diffusion behavior of these impurities as well as the host elements in CdTe has not been clearly understood. Using first-principles calculations, the diffusion behaviors of the cation atoms (Cd and Cu) and the anion atoms (Te and Cl) at different charged states are investigated. We find that, due to different electronic level occupations and level splittings, the diffusions of the cation atoms and anion atoms are very different. We explain why Cu can diffuse much faster than other elements and show that the diffusion speeds of the impurities can be controlled by tuning the Fermi level of CdTe. We have also developed a general diffusion coefficient theory for multi-barrier diffusion. Our calculated diffusivity of the interstitial impurities agrees well with available experimental measurements.

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