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Intermediate Band Formation in Selenium Doped Silicon ELIF ERTEKIN, JEFFREY GROSSMAN, Massachusetts Institute of Technology, COMPUTATIONAL NANOSCIENCE GROUP TEAM — The intermediate band solar cell is a promising approach to achieving high efficiency photovoltaic conversion, with theoretical limiting efficiencies in principle well exceeding those of conventional single gap semiconductors. The presence of an intermediate defect band within the normally forbidden band gap of the photovoltaic material allows the absorption of normally unused low energy solar photons. Using total energy electronic structure methods based on Density Functional Theory, we explore in detail the formation of a defect band as the concentration of Selenium defects in Silicon is increased from below to above the intermediate band transition limit. Two isolated defect states in Selenium, a double donor in Silicon, are observed. As the concentration of defects is increased, the localized defect states, with correspondingly flat bands, begin to overlap, resulting in electron delocalization and the formation of a continuous, dispersive defect band.

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