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Modeling and Study of Photovoltaic Materials Based on Density Functional Theory[1] ALEX CIMAROLI, WANJIAN YIN, TINGTING SHI, YANFA YAN, University of Toledo, NREL COLLABORATION — Understanding semiconductorproperties and defect states by use of Density Functional Theory (DFT) may allowmore efficient solar cells tobe made. According to calculations, intrinsic grain boundaries in CuInSeproduce deep gap states, and grain boundaries in CuZnSnSeact as Shockley-Read-Hall recombination centers. DFTwasused to aid in finding novel materials that have not been studied yet. Specifically, some of the Cu-V-VImaterials may prove to make good absorber layer materials aftercalculatingthe stability of different stoichiometries and their band gaps. The Al-O complex defect in Silicon is studied to understand its effect on the efficiency of Silicon solar cells. Some of the Al-O complexes produce deep levels in the band gap of Silicon, which reduces carrier lifetime. Lastly, Zinc Phosphide can grow preferentially along the [220] direction. DFT was used to calculate the surface energy of the different planes of Zinc Phosphide. The configurational energy should help to elucidate the nature of preferred orientation of Zinc Phosphide. (220)-oriented Zinc Phosphide thin films may have unique electronic and optical properties that can be explained by DFT.

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