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Localized states due to oxygen in II-VI semiconductors PAUL KENT, University of Cincinnati, CLAS PERSSON, Royal Institute of Technology Stockholm, ALEX ZUNGER, National Renewable Energy Laboratory — We study the electronic structure of dilute oxygen impurities in II-VIs (ZnTe, ZnSe, ZnS, CdTe, CdSe, CdS) using fully-relaxed large supercell density functional calculations. We analyze the ensuing localized electronic states, finding that oxygen induces "cluster states" (CS) near the conduction band edge, similar to nitrogen localized states in the III-Vs. In contrast to nitrogen in the III-Vs however, the CS in II-VI's exhibit a greater degree of delocalization owing to a greater hybridization with the host band structure. The fundamental character, origin, and energetic alignment of the CS is analyzed using the spectral projection method and hydrostatic pressure calculations. We discuss the ramifications of the CS on the band gap bowing, effective masses, absorption and emission spectra of dilute oxygen alloys.

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