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The electronic properties of point defects in earth-abundant photovoltaic material Zn_3P_2: A hybrid functional method study WAN-JIAN YIN, YANFA YAN, University of Toledo — Zinc phosphide (Zn_3P_2) is an attractive and promising semiconductor for thin-film solar cell application because of its earth abundance and ease of thin-film fabrication. The electronic properties of intrinsic and extrinsic defects in Zn_3P_2 are studied by density-functional theory with hybrid functional method. Our results show that undoped Zn_3P_2 should be intrinsically p-type with Zn vacancies as the responsible shallow acceptors. Na or Cu doping is expected to result in improved p-type conductivity as compared to intrinsic Zn_3P_2. S or Al doping may lead to weak n-type Zn_3P_2. Doping of Mg does not produce good n-type Zn_3P_2, consistent with experimental observations. Contradicting to conventional wisdom, an interstitial P in Zn_3P_2 is not a triple-hole acceptor and a P vacancy in Zn_3P_2 is not a triple-electron donor. Instead, we find that the interstitial P is actually a single-hole acceptor and the P vacancy is a single-electron donor. The origins of these unusual behaviors are discussed.

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