

Abstract Submitted
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AX centers in II-VI semiconductors: Hybrid functional calculations¹ KOUSHIK BISWAS, MAO-HUA DU, Materials Science and Technology Division, Center for Radiation Detection Materials and Systems, Oak Ridge National Laboratory — Group-V acceptors should be efficient hole producers in II-VI compounds as in ZnTe. However, good *p*-type conductivity remains elusive, for example in ZnO and ZnS. With regard to this low doping efficiency, we will discuss the dopant self-compensation in II-VI semiconductors through the formation of the AX center. These are acceptor-induced defect that acts as a donor to compensate the acceptor itself. We show that the artificially high valence band maximum in Local density approximation and Generalized gradient approximation calculations can lead to incorrect prediction on the stability of the AX center in these semiconductors. The hybrid functional calculations that correct the band gap, significantly stabilize the AX centers for selected group-V acceptor dopants in ZnO, ZnS, and ZnSe. The results on AX centers obtained by hybrid functional calculations agree well with the experimentally observed doping phenomena in ZnS and ZnSe.[1] [1] Koushik Biswas and Mao-Hua Du, Applied Physics Letters 98, 181913 (2011).

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