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First-principles study of point defects in κ-Al_2O_3 JUSTIN R. WEBER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The development of gate-stack structures for novel CMOS applications has stimulated interest in point defects that may occur in oxide dielectrics. We consider Al_2O_3 as a possible gate-stack material, and study defects in the low density κ phase. The choice of the κ-Al_2O_3 phase is based on the similarity of its density to that of amorphous Al_2O_3. We analyze native point defects such as vacancies, self-interstitials, and antisites, as well as various relevant impurities. Our first-principles calculations are based on density functional theory (DFT). Hybrid functionals were utilized as a means of overcoming the band-gap problem. This approach allows us to accurately assess the positions of defect levels. We use calculated band offsets to make predictions about the location of these defect levels with respect to the band gap of relevant semiconductors used as channel materials. We will discuss which defects may impede the optimal performance of devices.

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