Abstract Submitted
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Hybrid functional calculations for native defects and dangling bonds in α-Al_2O_3[1] MINSEOK CHOI, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Al_2O_3 is a promising material for use as a gate dielectric in III-V-based MOS devices, including in GaN-based transistors. Recent developments indicate that despite the relatively high structural quality, the presence of charge traps and fixed-charge centers near the interface between the oxide and nitride still poses serious problems for device performance. Native defects and dangling bonds in the Al_2O_3 dielectric or in the vicinity of the interface are the most likely causes. To aid in the identification of these centers, we perform density functional calculations with a hybrid functional for point defects and dangling bonds in α-Al_2O_3. We determine the position of the defect transition levels in the gap of the oxide, and analyze the level positions with respect to the nitride band edges. Our results show that O vacancies and Al dangling-bonds can produce charge traps and Al interstitials act as fixed charges in GaN-based n-MOSFETs.

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