

Abstract Submitted
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Impact of carbon and nitrogen on gate dielectrics in metal-oxide-semiconductor devices¹ MINSEOK CHOI, JOHN L. LYONS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Al_2O_3 and HfO_2 are used as alternative gate oxides in CMOS technology. Promising results have been achieved with Al_2O_3 /III-V and HfO_2 /Si MOS structures, which exhibit relatively low densities of interface states. However, the presence of charge traps and fixed-charge centers near the oxide/semiconductor interface still poses serious limitations in device performance. Native point defects are usually proposed as an explanation; unintentional incorporation of impurities in the gate dielectric during the deposition process has so far received less attention. Using first-principles calculations based on hybrid functionals we investigate the effects of carbon and nitrogen impurities in Al_2O_3 and HfO_2 . By analyzing the position of the impurity levels with respect to the III-V and Si band edges, we determine if these impurities can act as charge traps or sources of fixed charge. Our results show that carbon can act as a charge trap and lead to leakage current through the gate dielectric. Nitrogen can act as a source of negative fixed charge, but may be effective in alleviating the problem of charge traps and fixed charges associated with Al, Hf, and O vacancies.

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