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Carbon impurities in oxide dielectrics[1] HIRAL D. TAILOR, University of California, Santa Barbara , JOHN L. LYONS, Brookhaven National Laboratory, MINSEOK CHOI, Korea Institute of Materials Science, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara —
The high-k oxides ZrO_2, and $LaAlO_3$ can be used as dielectrics in metal-oxide-semiconductor (MOS) devices. Dielectrics are commonly grown with atomic layer deposition (ALD), often leading to unintentional incorporation of impurities such as carbon from the metal-organic precursors. Experiments indicated that carbon can be a significant cause of leakage current. We investigate this problem using density functional theory with a hybrid functional. Our results show that carbon substituting on the cation site undergoes an off-site displacement and forms close *sp* bonds with three oxygen atoms in ZrO_2 and $LaAlO_3$. We calculate the corresponding defect levels, and in order to determine the impact on MOS devices we align the band structures of the dielectrics with those of the semiconductor channel materials (including GaN, Si, and GaAs) . We find that carbon incorporation leads to defect levels near the conduction-band minimum of the channel materials, proving potentially detrimental for n-type devices. Intriguingly, we find that the defect levels of these carbon centers in a variety of oxides and semiconductors are aligned at roughly -3.5 eV below the vacuum level.

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Hiral D. Tailor
University of California, Santa Barbara

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