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Theoretical study of the insulator/insulator interface: band alignment at the SiO_2/HfO_2 junction ONISE SHARIA, ALEXANDER A. DEMKOV, The University of Texas — Hafnia has emerged as a front runner for replacing silica as a gate oxide in CMOS technology. One of the problems which still remains outstanding is finding a p-type gate metal for hafnia. Thus the problem of band alignment at the hafnia/metal and hafnia/Si interfaces has recently received significant attention. However, it is worth noting that during the deposition of hafnia on a silicon substrate a thin layer of silica is always created. And the band alignment between silica and hafnia can dramatically change the overall alignment across the gate stack. In this presentation we will discuss the band alignment at the SiO_2/HfO_2 interface. As we shall show it can be significantly different from the simple Schotky limit. We perform *ab-initio s*tudies of the interface using density functional theory in the local density approximation. We construct several atomic level models of the interface which connect hafnia to silica *via* an oxygen plane as required by the electron count rule that ensures the absence of electronic states in the gap. The models differ by the interfacial oxygen coordination, HfO_2 phases, and strain, and are fully relaxed. All interfaces can be categorized by the interfacial oxygen average coordination number. The calculated valence band offset varies from 1.0 eV to -2.0 eV and most strongly depends on the average coordination of the interface oxygen.

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