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Self-interaction corrected extrinsic levels of oxygen vacancies in hafnia GIORGIA M. LOPEZ, VINCENZO FIORENTINI, ALESSIO FILIPPETTI, SLACS-CNR and University of Cagliari, Italy — To identify fixed-charge (generally negative) centers in thin hafnia layers on silicon, the position and nature of the electronic levels of candidate defects should be known accurately. Due to the DFT gap problem, this is still a controversial issue in ab initio calculations, especially for high-gap insulators and near-conduction states. Here we apply a self-interaction corrected DFT method, which dealt successfully with a variety of systems dominated by localized and correlated states, to study the electronic structure of oxygen vacancies in monoclinic hafnium oxide in various charge states. We set the position of the extrinsic levels within the gap, and relative to the Si gap position as determined by interface band offsets. In the positive states, the partially filled levels are well below the Si gap, hence the Fermi level, and play a minor role. For the neutral vacancy, a filled extrinsic state sits within the Si gap and may tend to pin the Fermi level. A negative center may be realized upon occupation of a near-conduction shallow state, which would occur under typical device operation bias. While a conclusive identification of fixed-charge centers remains an open issue, the nature of this level is compatible with the experimentally observed kinetics of trapping and detrapping.

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