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Monolayer modification of interface dipoles between a-Al_2O_3 and silicon STEPHANIE FERNANDEZ-PEÑA, University of Geneva, A.M. KOLPAK, S. ISMAIL-BEIGI, C.H. AHN, F.J. WALKER, Center for Research on Interface Structures and Phenomena, Yale University, New Haven, Connecticut — Interface dipoles occurring at high-k oxide-silicon interfaces play an important role in the function of electronic devices. The magnitude and sign of the dipole depend sensitively on the chemistry of the first few atomic planes around the interface. In this work, we control the dipole between a-Al_2O_3 and silicon by monolayer modifications of interface chemistry. The interface composition ranges from a clean 2×1 Si (001) surface prepared by SiO desorption in ultra high vacuum to surfaces having thicknesses of SiO_x as thin as 1 monolayer. In these materials, we observe using x-ray photoelectron spectroscopy band-offset changes induced by a modified interface dipole as large as 0.4 eV. From the capacitance-voltage behavior of metal oxide semiconductor (MOS) devices, we find that this dipole responds to an applied electric field in a non-linear way. We understand this non- linear behavior using first principles theory of complex oxide- electrode interfaces.

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