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Core level shift and charge transfer of Sr templates on Si(001) for epitaxial oxide growth: theoretical and experimental study MIRI CHOI, AGHAM POSADAS, HOSUNG SEO, RICHARD HATCH, ALEXANDER DEMKOV, The University of Texas at Austin — Sub-monolayer Sr templates are used as a transition layer in the epitaxial growth of perovskite oxides on semiconductors. However, a detailed understanding of how the template enables oxide growth on Si(001) is still lacking. Sr on Si(001) shows different structural and electronic properties as a function of Sr coverage. Using a combination of *in situ* reflection high energy electron diffraction (RHEED) and *in situ* x-ray photoelectron spectroscopy (XPS), we observed both the Si 2p and Sr 3d core levels shift toward higher binding energy as Sr coverage increases up to one half monolayer. In addition, increase of Sr coverage leads to unbuckling of the Si dimer atoms as evidenced by the merging of the up and down dimer core level components as Sr donates charge to the dimer atoms. The work function of Si also shifts with Sr coverage as observed using ultraviolet photoelectron spectroscopy (UPS).

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