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First principles study of Al/$SrTiO_3$ interface formation ALI HAMZE, AGHAM POSADAS, KRISTY KORMONDY, ALEXANDER DEMKOV, Univ of Texas, Austin — Two-dimensional electron gasses (2DEGs) at the interfaces of oxides have been the subject of much interest in recent years due to their relatively high carrier mobilities and potential for use in all-oxide devices. In particular, the γ-Al_2O_3 (γ-alumina)-$SrTiO_3$ (STO) system has been the focus of much research. It exhibits a 2DEG at the interface with a carrier mobility ranging from 10^3-10^5 $cm^2\,V^{-1}\,s^{-1}$, depending on the thickness of the STO and how the γ-alumina film was grown. It is believed that Al atoms steal oxygen from the STO substrate at growth temperature and thus create a conductive channel in STO near the interface. We investigate the initial studies of the interface formation using density functional theory. The results of first principles calculations are compared with those of x-ray photoemission spectroscopy (XPS) performed in situ on thin Al films deposited on STO by molecular beam epitaxy. Analysis of the Al 2p XPS spectrum shows one layer of aluminum is fully oxidized during growth at 40C and 4 layers of aluminum are fully oxidized during growth at 600C. Furthermore, the Ti 2p XPS spectrum shows the titanium atoms are reduced, which is consistent with the presence of oxygen vacancies in STO.

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