The role of the $\sqrt{13} \times \sqrt{13} - R33.7^\circ$ surface reconstruction on superconducting FeSe/SrTiO$_3$ STEPHEN D. ALBRIGHT, Department of Physics and Center for Research on Interface Structures and Phenomena (CRISP), Yale University, K. ZOU, SUBHASISH MANDAL, DIVINE KUMAH, Department of Applied Physics and CRISP, Yale University, OMUR DAGDEVIREN, G.H. SIMON, UDO SCHWARZ, Department of Mechanical Engineering & Materials Science and CRISP, Yale University, ERIC ALTMAN, Department of Chemical & Environmental Engineering and CRISP, Yale University, MYUNG-GEUN HAN, YIMEI ZHU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, SOHRAB ISMAIL-BEIJI, F.J. WALKER, C.H. AHN, Department of Applied Physics and CRISP, Yale University — The creation of specific oxide surface structures is important to nucleating epitaxial growth. Here we show that the reconstructions of the SrTiO$_3$ (STO) surface impact the properties of monolayer FeSe grown on STO. We achieve high-quality epitaxial growth of FeSe on surfaces that feature a double TiO$_2$ termination, such as the $\sqrt{13} \times \sqrt{13} - R33.7^\circ$ reconstructed STO surface prepared by high-temperature annealing in oxygen. Diffraction patterns characteristic of the reconstruction are observed with electron and synchrotron x-ray diffraction. The detailed structure of the FeSe/$\sqrt{13} \times \sqrt{13} - R33.7^\circ$ interface is determined using crystal truncation rod analysis, and the double TiO$_2$ termination observed is consistent with previous transmission electron microscopy studies. We further demonstrate the significance of this particular interface structure on epitaxial growth and its implications for the resulting electronic structure using first principles theory.

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