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Role of double TiO_2 layers at the FeSe/$SrTiO_3$ superconducting interface: A Density functional study[1] S. MANDAL, Department of Applied Physics, Yale University, R. PENG, Y. PU, D. FENG, Department of Physics and Advanced Materials Laboratory, Fudan University, X. HE, I. BOZOVIC, Brookhaven National Laboratory, K. ZOU, S. ALBRIGHT, G. SIMON, O. E. DAGDEVIREN, U. D. SCHWARZ, E. I. ALTMAN, D. KUMAH, F. J. WALKER, C. H. AHN, S. ISMAIL-BEIGI, Center for Research on Interface Structures and Phenomena (CRISP), Yale University — The recent discovery of high temperature superconductivity in monolayer FeSe on $SrTiO_3$ (STO) has drawn much attention. Since there is a strong enhancement of superconductivity compared to bulk FeSe, understanding the interfacial interactions between FeSe and STO is important. To date, density functional theory (DFT) studies have had difficulties explaining a key feature in the observed Fermi surface topology: namely the absence of a "hole pocket" about the Γ point in the Brillouin zone of the heterostructure. By combining DFT and experiment, we find that the STO surface termination is not the primitive $1\times$ 1 single-layer TiO_2 assumed in most works but instead is a more complex double-layered TiO_2 structure. We find that the double layer facilities epitaxial growth of monolayer FeSe. Our DFT calculations show that the hole pocket can be eliminated by the enhanced tendency of the double layer (compared to the single layer) termination to donate electrons to the FeSe when oxygen vacancies are present at the STO surface.

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