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The role of double TiO₂ layers at the interface of FeSe/SrTiO₃ superconductors

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The marked enhancement of the superconducting critical temperature for FeSe grown on SrTiO₃ (STO) is a notable recent discovery in the field of high temperature superconductivity. A complete understanding of the mechanism for this enhancement has not been elucidated and is thought to be due to how the electronic structure is modified by the interface. We determine the surface reconstruction of SrTiO₃ that is used to achieve superconducting FeSe films in experiments. In particular, we observe the existence of a double TiO₂ layer and identify the symmetry of the reconstruction at the FeSe/SrTiO₃ interface. The double TiO₂ layer plays two important roles. First, it facilitates epitaxial growth of FeSe films. Second, *ab initio* calculations reveal that electron transfer to the FeSe is enhanced by the double layer termination more strongly than by other surface structures of SrTiO₃. The enhanced electron transfer suppresses the hole pocket near the Γ point, leading to a band structure characteristic of superconducting samples. The characterization of the interface structure presented here is a key step towards understanding the electronic properties of this novel superconductor.