

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Defects in Thin-Film FeSe/SrTiO₃: STM and DFT Investigations¹ DENNIS HUANG, Harvard University, TATIANA A. WEBB, University of British Columbia, Harvard University, CAN-LI SONG, Tsinghua University, CUI-ZU CHANG, JAGADEESH S. MOODERA, Massachusetts Institute of Technology, EFTHIMIOS KAXIRAS, Harvard University, JENNIFER E. HOFFMAN, University of British Columbia, Harvard University — A single-layer of FeSe deposited on SrTiO₃ exhibits an order-of-magnitude enhancement of its superconducting transition temperature compared to bulk FeSe. This dramatic effect is curiously absent in a second layer of FeSe deposited on the heterostructure, leading to many questions concerning the role of the interface structure, electron doping and phonon coupling. Here, we approach these questions by using STM to characterize and compare native defects that appear in multi-layer and single-layer FeSe/SrTiO₃ grown by MBE under excess Se flux. We use DFT to explore candidate defect configurations, formation energies and diffusion barriers, in order to gain atomic-scale insights into the growth and structure of these film heterostructures.

¹Work supported by NSF DMR-1231319 (STC CIQM) and Moore Foundation EPiQS GBMF4536. Computations run on Harvard RC Odyssey.

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Date submitted: 05 Nov 2015

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