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Effects of interface oxygen vacancies at the FeSe/$SrTiO_3$ interface
MINGXING CHEN, D. F. AGTERBERG, L. LIAN, MICHAEL WEINERT, Univ of Wisconsin, Milwaukee — The effects of oxygen vacancies on the electronic bands at the interface of between monolayer and bilayer FeSe and $SrTiO_3$ are investigated by first-principles supercell calculations. Unfolded bands derived from the k-projection method reveal that the oxygen vacancy not only provides electron doping to the interface FeSe layer, but also significantly renormalizes the width of the Fe-3d band near the Fermi level for the checkboard antiferromangetic (AFM) state. However, the effects of the oxygen vacancies on the electronic properties of the top layer of bilayer FeSe are limited. The k-projected bands for the checkboard AFM state are in good agreement with ARPES results.

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