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Final-state effect on X-ray photoelectron spectrum of n-doped SrTiO₃¹ CHUNGWEI LIN, AGHAM POSADAS, ALEXANDER DEMKOV, UT Austin, Physics Department, DEMKOV TEAM — X-ray photoelectron spectroscopy (XPS) is a widely used technique to determine the oxidation states of chemical elements. In stoichiometric SrTiO₃, the Ti⁴⁺ peak appears at a binding energy of about 459.0 eV for photoelectrons ejected from the Ti 2*p* core level. In lightly n-doped SrTiO₃, a weak shoulder at a binding energy of about 1.5 eV lower than the Ti⁴⁺ peak appears in the XPS spectrum that has been conventionally interpreted as a Ti³⁺ signal. By taking the final-state effect into account, i.e. by considering the response of the valence electrons in the presence of a core hole, we argue that such a Ti³⁺ peak does not necessarily imply the existence of spatially localized Ti³⁺ ions, and explicitly show that a spatially uniform Ti^{(4-x)+} distribution also leads to the multi-peak structure. Spectra from metallic n-doped SrTiO₃ (e.g. La replacing Sr, Nb replacing Ti, or even oxygen vacancy doping) should be interpreted as the latter case. Several experiments based on this interpretation are discussed.

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Chungwei Lin
UT Austin

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