

$k \cdot p$ subband structure of the $\text{LaAlO}_3/\text{SrTiO}_3$ interfaceL. W. van Heeringen¹, G. de Wijs, A. McCollam, J. C. Maan and A. Fasolino*Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands*¹ *l.vanheeringen@science.ru.nl*

A high-mobility electron gas at the $\text{SrTiO}_3/\text{LaAlO}_3$ interface [1] showing multisubband Shubnikov-de Haas oscillations with a few meV subband separation has been observed [2]. We analyze these results by calculating the subband structure in the 6-band $k \cdot p$ envelope function approach with an electric field confining the electron gas in the SrTiO_3 at the interface. By fitting to DFT band structure calculations we determine the 5 relevant parameters: 3 effective mass parameters for the t_{2g} conduction band edge (d_{xy} , d_{yz} and d_{zx}) of SrTiO_3 , the spin-orbit coupling and the low temperature tetragonal distortion. The electric field strength F is treated as a variable since we do not incorporate lattice and electron screening in our model. This model leads to anisotropic non-parabolic bands as in Fig. 1. Similar band structures result from tight binding calculations in the ‘low density regime’[3].

This model allows a direct comparison to the frequency of the quantum oscillations observed in high magnetic fields through quasiclassical quantization for a given density. Our results are in good agreement with the experiments for an electric field strength $F = 0.1 \text{ meV/\AA}$ and a density of $7.1 \times 10^{12} \text{ cm}^{-2}$.

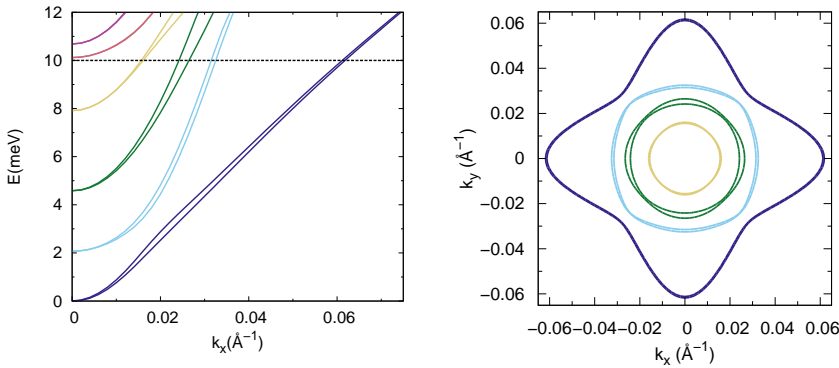


Figure 1: Left: SrTiO_3 subbands in an electric field of $F = 0.1 \text{ meV/\AA}$. The small spin splittings are due to the asymmetric well in presence of spin-orbit coupling. Right: corresponding equal energy contours at $E = 10 \text{ meV}$. Note the highly non-parabolic and anisotropic nature of the subbands.

[1] A. Ohtomo, H. Hwang, *Nature*, **427**, 204 (2006).

[2] A. McCollam, S. Wenderich, M. K. Kruize, V. K. Guduru, H. J. A. Molegraaf, M. Huijben, G. Koster, D. H. A. Blank, G. Rijnders, A. Brinkman, H. Hilgenkamp, U. Zeitler, J. C. Maan, *arXiv:1207.7003* (2012).

[3] G. Khalsa, A. H. MacDonald, *Phys. Rev. B*, **86**, 125121 (2012).