Band Dispersion within Pristine InBi Crystal

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Abstract. InBi has been theoretically analysed for many years as a semi-metal showing a stable phase within the PbO structure thanks to Spin-Orbit Coupling (SOC) forces [1,2,3]. Regrettably, this alloy system remains not well-known on the experimental side: reports of grown ordered crystals are rare [4,5]. We here present a thorough experimental and *ab-initio* theoretical analysis on InBi(001).
The crystal was grown using the Bridgman–Stockbarger technique. InBi consists of In layers sandwiched between Bi monolayers, with weak Van-der-Waals bonds amid the resulting trilayers. The InBi crystal was cleaved *in-situ* in order to obtain a clean and flat surface suitable for angle-resolved photoemission (ARPES) measurements.
The SPR-KKR package [6,7], based on the Dirac equation, which fundamentally includes relativistic effects, was used for the theoretical analysis and clearly underlines the influence of the surface termination.

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