ARPES Studies of Hf(0001) Surface: Flat Bands Formation in the Dice Lattice

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Abstract. We present the first electronic structure measurements of the Hf(0001) single-crystal surface using angle-resolved photoemission spectroscopy (ARPES). The ARPES results are supported by theoretical calculations performed using the full-potential linearized augmented plane wave (FLAPW) method and the Korringa-Kohn-Rostoker (KKR) Green function method. In addition to insight into the electronic structure of Hf(0001), our results reveal the impact of surface contamination, particularly oxygen and carbon, on the predicted surface state. Moreover, we observe a flat band induced by both, the presence of oxygen and the dice structure of the surface. The orbital texture of Hf bands is confirmed by linear dichroism studies.