Influence of Hf (0001) Surface Contamination on ARPES: a DFT Study Supporting Experiments

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Abstract. We present first ARPES studies of the electronic structure of the Hf(0001) surface. High-Z materials have attracted much interest, because the strong spin-orbit coupling in combination with the broken inversion symmetry and an important effective electric field at the surface results in a spin-momentum locking. Spin-polarized electrons at the surface are of interest in physics and novel applications in electronics and data processing. Extra sharp peaks observed in experiment are identified thanks to ab-initio calculations performed within the SPRKKR package. These extra states come from oxygen contamination of the highly reactive surface of Hf(0001). Further comparison is done on the ARPES level, thanks to the one-step model which include all matrix elements effect, resulting in an excellent agreement.