Electronic supplementary information (ESI) for:

Effect of Au/HfS₃ interfacial interactions on properties of HfS₃-based devices

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Figure S1. Band diagrams under different scenarios. (a) n-type HfS_3 in vacuo (left) versus ptype HfS_3 in air (right). O₂ chemisorption pushes the n-type Fermi level (E_F) downwards (closer to its valence band) to make it p-type. The physics of band bending for (b) n-type Schottky barrier at the Au/HfS₃ interface, and the physics of band bending for (c) p-type Schottky barrier at the Au/HfS₃ interface. Due to chemisorption of O₂, the E_F of HfS₃ is pushed downwards leading to an increase in its work function. Consequently, a p-type Schottky barrier is formed at the Au/HfS₃ interface, implied by downward band bending. This downward band bending manifests itself as an equivalent increase in the binding energies of the sulfur and hafnium XPS core-levels (shown in Fig. 3b and 3c of the main text).