Emergence of Flat Bands in Solids: Case of Hf(0001)

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Abstract. Flat bands are unique features of the electronic structure that have recently garnered significant attention as fertile grounds for exploring rare quantum states. In the non-dispersive nature of massive bands, the electrons slow down almost to a halt enabling electronic correlation effects and resulting in ferromagnetism, high-temperature superconductivity or high-temperature fractional quantum Hall effect [1,2]. Flat band-hosting crystal lattices were theoretically proposed almost 40 years ago in the so-called dice structure [3] and later in many other models, such as Kagome, Lieb, pyrochlore or the Penrose tiling. In recent years, this field of physics has been stimulated by the identification of flat electronic bands in 2D moiré heterostructures [1].

Our LEED pattern on Hf(0001) indicates that the surface can, in fact, harbour the dice structure [1,3,4]. The stacking of two top Hf layers and the adsorbed oxygen layer leads to three atoms in the unit cell which is characteristic of the dice lattice [5]. Our observation of the flat band can then be attributed to the adsorption of oxygen (or carbon monoxide) molecules present in the residual gases of the UHV system. The similar system, CO/Cu(111), is used as a model for theoretical studies of electronic properties of the dice structure and it has been shown that CO acts as a repulsive barrier to surface electrons [4]. In this case a flat band is appearing at the Fermi level, but in their tight-binding calculation only s-bands have been involved. In our situation p- and d- orbitals are present that can modify the biding energy. Moreover, 5d atoms may lead to a flat band with strong spin-orbit coupling and lifting the spin degeneracy [6].

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