STM/STS studies of single-atom Fe inclusions in MBE-grown monolayer MoS_2/Gr/Ir(111)

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Transition metal dichalcogenides (TMDs) have drawn significant attention due to their scalability and the thickness-dependence of their electronic density of states (DOS) [1-2]. Moreover, dimensionally confined TMDs, mainly 2D monolayers (MLs), are highly sensitive to structural defects, such as vacancies, interstitial and substituent atoms. Even in very low-density regimes, these impurities significantly affect various properties by introducing stress and/or modifying the DOS [3-5]. Consequently, there are ongoing efforts to engineer defects in TMDs to tune their electronic, magnetic, optical, and catalytic properties. While most of the current research focuses on naturally occurring defects in chemical vapor deposited TMDs, to improve control over defect engineering, we focus on intentional single-atom inclusions in TMDs grown by molecular beam epitaxy (MBE).

In this presentation, I summarize our scanning tunneling microscopy (STM) and spectroscopy (STS) studies of Fe inclusions in ML MoS_2 on Gr/Ir(111), which we realize by co-evaporating Fe during MoS_2 MBE growth. We identify the Fe inclusions upon comparison with naturally occurring defects found on the undoped MoS_2 grown previously in the same UHV chamber. STS experiments reveal the presence of in-gap states arising from the incorporation of Fe atoms, whose spatial distributions are imaged by means of bias-dependent differential conductance mapping. Furthermore, resonant tunneling spectroscopy shows that the image potential states (IPS) are modified by the Fe inclusions, influencing the IPS' energetic positions due to a variation in the local work function.

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