

SINGLE-ATOM FE INCLUSIONS IN MBE-GROWN MONOLAYER MoS₂/GR/Ir(111): AN STM/STS STUDY

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Transition metal dichalcogenides (TMDs) have attracted considerable interest due to their tunable electronic structure and strong sensitivity to defects in the two-dimensional limit [1–4]. In monolayer TMDs, even low concentrations of vacancies, interstitials, or substitutional atoms can strongly modify local strain and the electronic density of states, providing opportunities for defect engineering of electronic, magnetic, optical, and catalytic properties. While most studies have focused on native defects in chemically grown materials, molecular beam epitaxy (MBE) enables controlled incorporation of designed atomic-scale impurities.

In this presentation, I discuss scanning tunneling microscopy and spectroscopy studies of intentionally introduced Fe inclusions in MBE-grown monolayer MoS₂/Gr/Ir(111), realized by co-evaporation of Fe during growth. The Fe-related defects are identified through comparison with intrinsic defects observed previously in undoped MoS₂ grown in the same UHV chamber. Differential conductance spectroscopy reveals impurity-induced in-gap states associated with Fe incorporation, while bias-dependent conductance mapping resolves their spatial structure. Resonant tunneling spectroscopy further shows that Fe inclusions modify image potential states, shifting their energetic positions through local variations of the work function. These results demonstrate controlled atomic impurity engineering in MBE-grown TMDs and its impact on the local electronic structure.

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