The influence of native defects on the electronic structure of CVD grown MoS_2 and $MoSe_2$ single layers

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2D layered nanomaterials like transition metal dichalcogenides (TMDCs) have attracted increased interest. These new materials possess electronic structures completely different from that of graphene, thus offering a wide range of physical properties. We have investigated MoS_2 and $MoSe_2$ sheets grown by chemical vapour deposition (CVD) on highly ordered pyrolytic graphite (HOPG) as a model system of heterostructures with atomically clean interface. [1] Our STM study revealed that the crystallographic orientation of TMDC sheets is determined by the orientation of the underlying graphite lattice. The electronic properties of the flakes have been investigated using tunnelling spectroscopy. A significant modification of the electronic structure has been revealed at flake edges and grain boundaries. We identified mirror twin grain boundaries (MTBs) and investigated the influence of their orientation relative to the zigzag directions of the lattice. These features are expected to have an important influence on the performance of nanoelectronic devices and catalytic activity of the nanostructures. Atomic resolution STM investigations also revealed a high density (10^{12} cm^{-2}) of native point defects. [2] Our DFT calculations predict that Mo vacancies in $MoSe_2$ are magnetic, and their magnetic moment can be efficiently tuned by tuning the Fermi level position. We have also demonstrated the ability of the STM to define nanoribbons down to 12 nm width, which can be used as building blocks for future nanoelectronic devices.

References

[1] A. A. Koós, et al.: Carbon 105 (2016) 408-415
[2] János Pető, et al.: Nat Chem. 10 (2018) 1246-1251

Figures

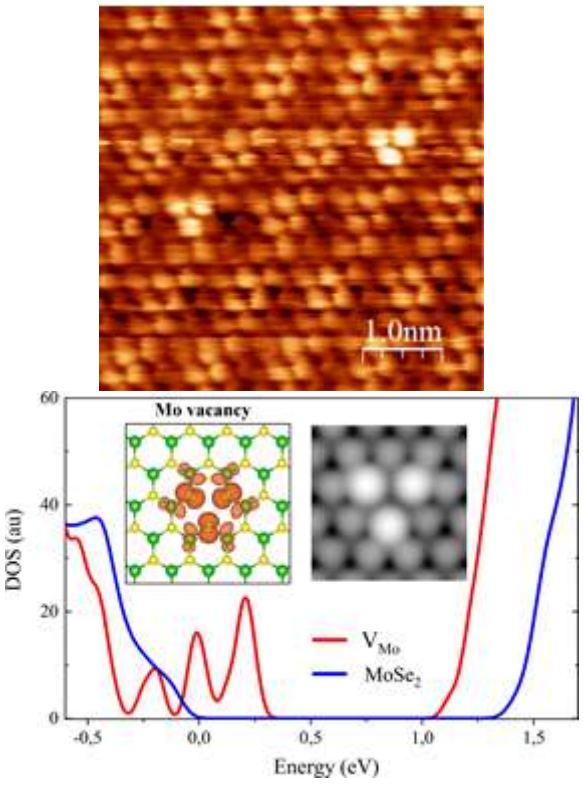

Figure 1: Atomic resolution STM image of point defects in MoSe2 and simulated STM image of Mo vacancy.