Electronic and Optical Properties of Defects in Transition Metal Dichalcoginide Monolayers

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Properties of two-dimensional (2D) transition metal dichalcogenides (TMDs) are highly sensitive to the presence of defects, and a detailed understanding of their structure may lead to tailoring of material properties through 'defect engineering'. Defects in 2D semiconductors are expected to substantially modify material properties. 2D TMD semiconductors are particularly interesting because they exhibit direct bandgaps in the visible range, high charge-carrier mobility, extraordinarily enhanced light–matter interactions, and potential applications in novel optoelectronic devices.

We have investigated the structural and electronic properties of point and 1D defects in $MoSe_2$ and WSe_2 TMD monolayers through atomically resolved low temperature STM/AFM imaging and spectroscopy [1]. We have also performed scanning near-field photoluminescence hyperspectral imaging of MoS_2 monolayers [2] to image optoelectronic properties at the 40 nm length scale.

The structure and electro-optic properties of mirror-twin domain boundaries and of several types of TMD point defects will be presented and discussed.

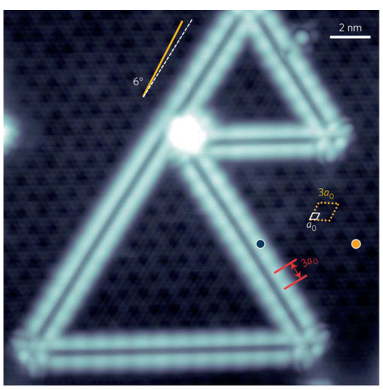

Figure 1 LT-STM image of $MoSe_2$ conductive mirror-twin domain boundaries. Charge density wave order has been identifed at low temperature [1].

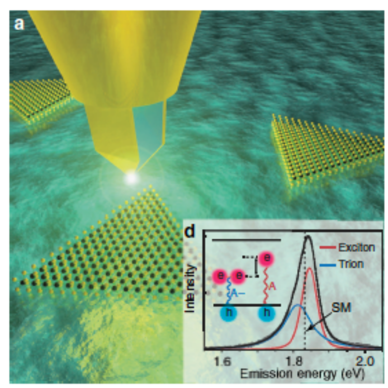

Figure 2 Scanning near field hyperspectral PL images of MoS_2 resolve excition and trion contributions to luminescence at the intrinsic lenght scales of CVD grown islands [2].

[1] Sara Barja, Sebastian Wickenburg, Zhen-Fei Liu *et al.*, Nature Physics <u>12</u> 751(2016).

[2] Wei Bao, Nicholas J. Borys , Changhyun Ko *et al.*, Nature Communications <u>6</u> 7993 (2015

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The combination of STM imaging, STS spectroscopy and nc-AFM imaging provides detailed information on the electronic and geometric structure of both extended and point defects. Figure S1 shows STM (a) and nc-AFM (c) images of a mirror-twin boundary, along with image cross sections (b,d). Figure S2 shows STM and nc-AFM images of an S-vacancy point defect on the "top" of a WS_2 monolayer. "Bottom" S vacancies have also been identified [S1].

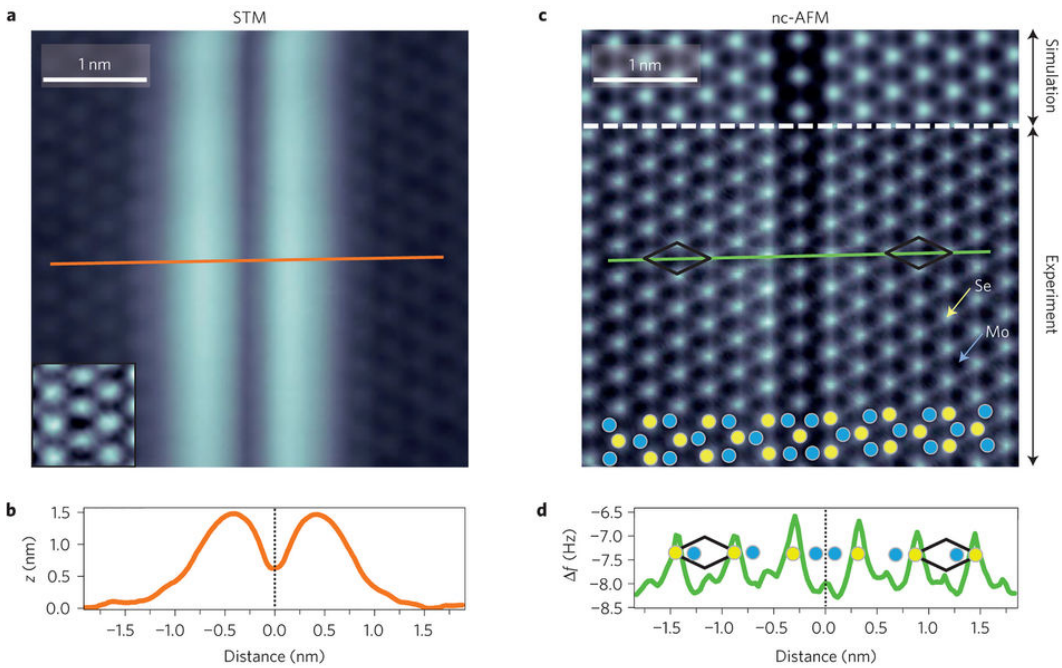

Figure S1. STM electronic structure and nc-AFM atomic structure of mirror-twin domain boundaries on $MoSe_2$. Knowledge of atomic structure provides a necessary input for theoretical evaluation of electronic structure [1].

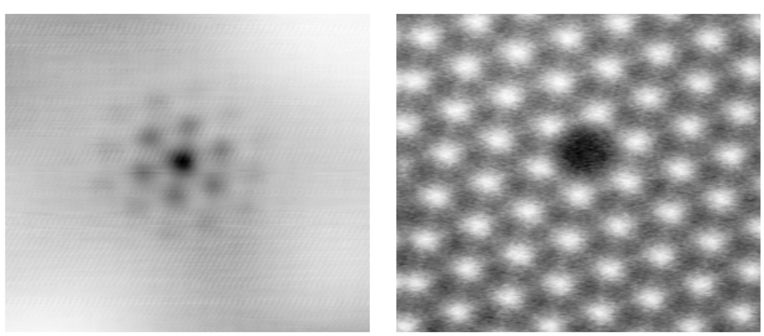

Figure S2. Scanning Tunneling Spectroscopy (+1.1 V) and nc-AFM images of a sulfur "top" vacancy in WS_2. [S1].

[S1] B. Schuler *et al*. To be published.