Gap Tuning by Hole Doping in $EuZn_2As_2$ Semimetal

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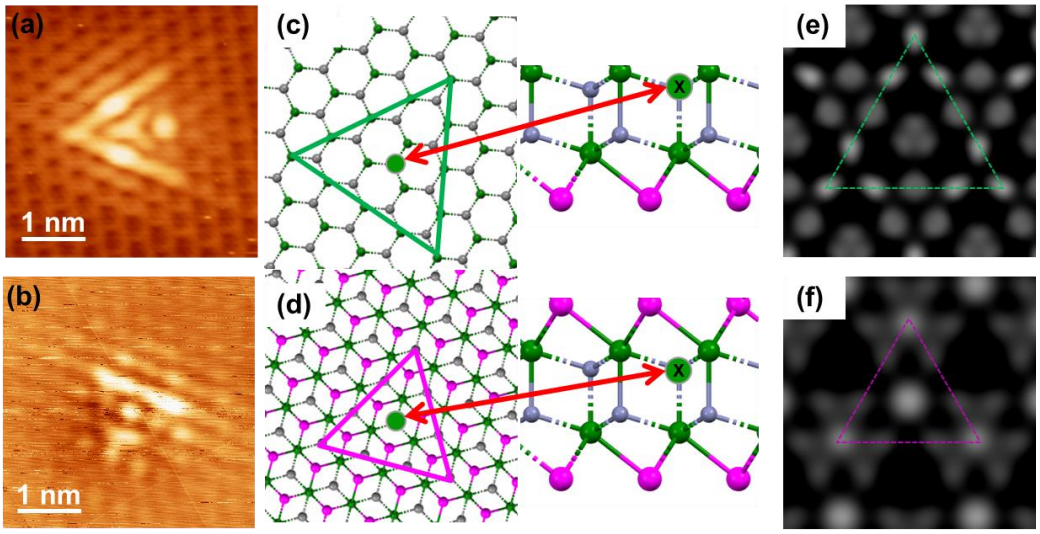

Figure 1. STM images of the substitutional defect on (a) As-terminated and (b) Eu-terminated surfaces. (c) and (d) Top view and side view of the structure models of the two defects. (e) and (f) The simulated STM images based on the DFT calculation of the corresponding defects.

$EuZn_2As_2$ is an ideal candidate for topological magnetism study in comparison to other europium-based semimetals that exhibit a similar type of magnetic transition from the antiferromagnetic phase to the ferromagnetic phase at a low temperature. [1] Theoretical calculations predict gapped and flatter bands in $EuZn_2As_2$ but a gapless Γ point in $EuCd_2As_2$. [2] In

this work, a low-temperature cleaved $EuZn_2As_2$ crystal is studied using scanning tunneling microscopy/spectroscopy (STM/S) and density functional theory (DFT). A group of triangular-shaped defects in combining with the DFT calculations are used to identify the existence of the europium-terminated and arsenic-terminated surfaces at the cleavage. Large bandgaps are observed on the two pristine terminations. However, the bandgap width is found to be very sensitive to local heterogenous, like defects and step edges. Two defect groups that create local electron deficiency, i.e. substitutional defect of As replacing Zn, and Zn vacancy, can drastically lower the bandgap. Furthermore, the modification of the bandgap width shows a discrepancy on the two terminations, bigger on Eu termination but much smaller on As-Zn termination. So, we predict that purposely hole doping the system during the crystal growth stage may create a new topological semimetal material with a gapless europium layer sandwiched by a gapped As-Zn lattice.

Reference:

1 Blawat, J. *et al.* Unusual Electrical and Magnetic Properties in Layered EuZn2As2. *Adv Quantum Technol* **5** (2022).

2 Wang, Z. C. *et al.* Anisotropy of the magnetic and transport properties of EuZn2As2. *Phys Rev B* **105** (2022).