Decoupling Molybdenum Disulfide from its Substrate by Cesium Intercalation

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Abstract

Intercalation of alkali atoms within the lamellar transition metal dichalcogenides is a possible route toward a new generation of batteries. It is also a way to induce phase transitions of interest for optical and electrical switches. The process of intercalation has been mostly studied in three-dimensional dichalcogenide films [1].

We will focus on single-layer of molybdenum disulfide (MoS_2), deposited on a gold substrate, intercalated with cesium (Cs) atoms in ultra-clean conditions (ultrahigh vacuum), in the form of a AuCs alloy [2]. Our work combines scanning tunneling microscopy, synchrotron X-ray diffraction, photoemission spectroscopy, and density functional theory calculations.

Intercalation is found to decouple MoS_2 from its substrate, increasing the spacing distance by fractions of a nanometer, and suppressing the modulations of its electronic properties that are associated with the MoS_2/Au(111) moiré pattern. Electron transfer occurs from Cs to MoS_2, the energy of the valence band maxima change, and electronic disorder is induced by structural disorder in the intercalated Cs layer. Besides, an abnormal lattice expansion of MoS_2 is found. Intercalation is thermally activated, and so is the reverse process of de-intercalation. Our work gives microscopic understanding on a process of relevance in several possible future technologies, and shows the way to the manipulation of the properties of two-dimensional dichalcogenides by "under-cover" functionalization.

References

[1] R. Friend & A. Yoffe, Adv. Phys. 36 (1987) 1
[2] R. Sant et al., under review.

Figures

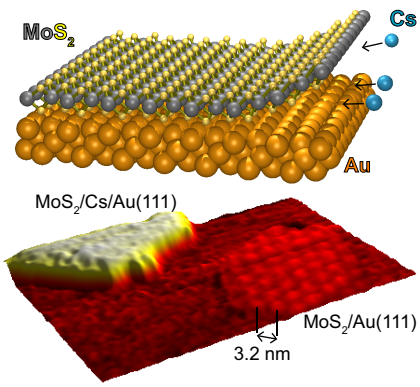

Figure 1: Cartoon illustrating the intercalation process between a single layer MoS_2 and its growth substrate, Au(111) (top). Scanning tunneling topography of single-layer MoS_2 islands, one intercalated with Cs and the other not (bottom).