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 (MoS2), 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 MoS2 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 MoS2/Au(111) moiré pattern. Electron transfer occurs from Cs to MoS2, 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 MoS2 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 MoS2 and its growth substrate, Au(111) (top). Scanning tunneling topography of single-layer MoS2 islands, one intercalated with Cs and the other not (bottom).