Investigation of the atomic and electronic structure of the van der Waals heterostructure $MoSe_2$-graphene

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In the route to novel functionalities of two-dimensional (2D) materials, three-dimensional entities conceptualized from 2D-lego pieces have drawn particular attention because of the dimensionality effect and exotic properties [1,2]. As 2D layers are held together by a van der Waals (vdW) force, vertical heterostructures based on these layers are a genuine approach which offers a fertile platform to study fascinating van der Waals-driven properties: commensurate lattice coincidence, electronic structure and band structure line-up, spin-orbit coupling induced by proximity effect and by inversion symmetry breaking.

In this poster, we report on the synthesis and characterization of the van der Waals heterostructure: $MoSe_2$/free-standing-graphene by molecular beam epitaxy. This fabrication approach consists of depositing $MoSe_2$ on graphitized graphene-SiC substrate, leading to a pure vdW interface. This enables to study properly the intrinsic properties as well as vdW-type interactions in this 2D system. We employed surface-sensitive techniques in order to probe structural and electronic properties of the heterostructure ranging from atomic resolution (STM-STS) to microscopic scale (synchrotron diffraction, ARPES). At the atomic standpoint, the STM shows point defects and twin boundaries in the $MoSe_2$ layer. This kind of defects is in general observed in MBE-2D layers due to Se vacancies and domain merging. STS measurement at selected point on $MoSe_2$ layer indicates a band gap of 2.1 eV separating the valence band maximum and conduction band minimum. Regarding the microscopic scale measurements, we found that the crystallographic directions of the $MoSe_2$ lattice align perfectly along the ones of graphene, resulting in only one commensurate configuration. This structural analysis by synchrotron diffraction is well consistent with the constant energy map in k-space of the electronic band structures of $MoSe_2$-graphene probed by ARPES. We observe a clear evolution of the band structure of the graphene-heterostructure compared to the one of bare graphene, which is a direct consequence of the interlayer coupling between the $MoSe_2$ layer and graphene. Finally, substrate-induced interactions will be also discussed by comparing the resulting data with the MBE-$MoSe_2$/graphene grown by chemical vapour deposition on $Pt/SiO_2/Si$ substrate.

References

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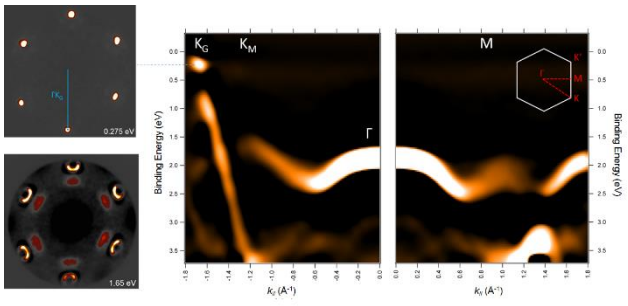

(a) (b)

Figure 1: ARPES constant energy maps (a) and band structure (b) of $MoSe_2$-Graphene viewed along the K-Γ-M direction of $MoSe_2$