Local, Intercalation Driven, Merging and Work Function Change of Epitaxial MoS_2 Grown on Graphene/Ir(111)

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Two dimensional (2D) materials and in particular transition metal dichalcogenides (TMDs) hold many interesting and novel physical properties that have attracted extensive research in the field.[1] From this family certainly the most studied one is 2D molybdenum disulfide, MoS_2, due to its widespread previous use, stability, flexibility and interesting electronic structure[2–5]. Even more interesting is layering 2D materials in heterostructures where one takes the advantages of the individual component to create a superior composite. Here we grow single layer MoS_2 on Gr/Ir(111) substrate in UHV conditions, thus forming a MoS_2/Gr heterostructure. We show that there is previously unreported local variation in MoS_2 growth creating two main types of regions: (a) areas with merged MoS_2 islands surrounded by larger areas of uncovered graphene in the vicinity of graphene wrinkles, and (b) areas with isolated, well defined, approximately equally spaced MoS_2 islands further away from wrinkles. We find through Kelvin probe force microscopy (KPFM) measurements that the work function of these areas differ, and connect the change to the local intercalation of Sulphur near graphene wrinkles. Our preliminary DFT calculations show that the S intercalated MoS_2 is more weakly bounded than non-intercalated islands resulting thus in their higher mobility and merging during growth. Our work highlights an importance of determining homogeneity of the sample on a larger scale but also shows a possible pathway for band structure and molecular adsorption engineering of TMDs.

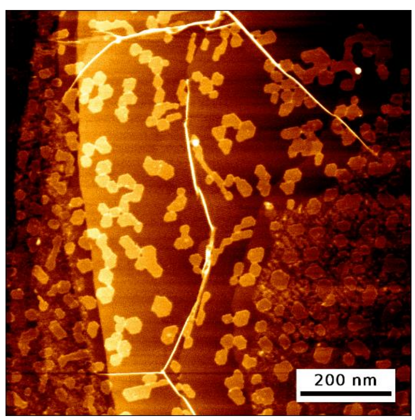

Fig. 1. AFM topography of MoS_2 on Gr/Ir(111).

1. Manzeli, S., Ovchinnikov, D., Pasquier, D., Yazyev, O. V. & Kis, A. 2D transition metal dichalcogenides. *Nat. Rev. Mater. 2017 28* **2**, 1–15 (2017).
2. Li, X. & Zhu, H. Two-dimensional MoS2: Properties, preparation, and applications. *J. Mater.* **1**, 33–44 (2015).
3. Akinwande, D., Petrone, N. & Hone, J. Two-dimensional flexible nanoelectronics. *Nat. Commun. 2014 51* **5**, 1–12 (2014).
4. Mak, K. F., Lee, C., Hone, J., Shan, J. & Heinz, T. F. Atomically Thin MoS_{2}: A New Direct-Gap Semiconductor. *Phys. Rev. Lett.* **105**, 136805 (2010).
5. Radisavljevic, B. & Kis, A. Mobility engineering and a metal-insulator transition in monolayer MoS_2. *Nat. Mater.* **12**, 815–20 (2013).