Interaction between 2D transition metal dichalcogenides and metal atoms for use in electrical contacting, investigated via experimental and simulated atomic resolution HAADF Scanning Transition Microscopy

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Effective contacting of 2D materials will be vital in these materials available for industrial applications, especially for the electronics industry. 2D forms of transition metal dichalcogenides (TMDCs) are attractive for electronics due to their bandgap characteristics. However, use of these 2Ds by the electronics industry will be unattainable unless a stable electrical contacting solution can be found.
DFT calculations and theoretical studies from multiple sources have suggested various metals that might form favourable contacts with TMDCs [1]. AFM and Raman spectroscopy has also been used to characterize metals when grown or transferred to thin films [2]. However, there is sparse experimental evidence of the detailed interaction, i.e., on the atomic level.

The distribution and characteristics of gold on the transition metal dichalcogenides MoS_2 is being investigated using atomic resolution high angle annular dark field (HAADF) imaging. MoS_2 was physically exfoliated to create thin, few-layer areas. Introduction of angstrom quantities of metals on the flakes allow for the interaction of the metal and TMDC to be investigated on the sub-Å scale in an aberration-corrected transmission electron microscope. Simulations of HAADF STEM images of a gold particle on monolayer MoS_2 were created for comparison to experimental images, to attempt to gain an accurate view of the size and agglomeration of the gold on the MoS2 surface. Models varying the number of gold atoms and atomic structure were created to find the closest match to the experimental observed gold nanoparticles.

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1. Kang, J., Sarkar, D., Liu, W., Jena, D. & Banerjee, K. A computational study of metal-contacts to beyond-graphene 2D semiconductor materials. in *2012 International Electron Devices Meeting* 17.4.1-17.4.4 (IEEE, 2012). doi:10.1109/IEDM.2012.6479060
2. Cho, S. *et al.* DEVICE TECHNOLOGY. Phase patterning for ohmic homojunction contact in $MoTe_2$. *Science* **349,** 625 - 8 (2015).