THEORETICAL STUDY OF MoS_2 CONTACTS MODES WITH METALS

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In the near future, the manufacturers of logic transistors will face the inevitable failure of the present technology to fulfill the Moore's law requirement below 20 nm line width. The solution is to go down in scale until the fundamental limit of a single atom layer. Recently, a large variety of 2D materials, including graphene and single atom layers of rhodium and palladium, has been synthesized. However, these materials do not have a bandgap.

Molybdenum disulfide, a widely studied semiconducting layered transition metal dichalcogenide, possesses an indirect band gap of 1.3 eV in bulk and a direct band gap of 1.9 eV in the monolayer [1]. Several studies [2, 3] have reported large resistance between contacts and semiconducting layer. It shows us the importance of more thorough research of metal-mTMD (monolayer transition-metal dichalcogenide) edge contacts. The experimental comparison has been presented between the basal (top) and edge planes of MoS_2 by using macroscopic molybdenite crystals [4]. On selective exposure of only the basal or edge plane, a comparison of their electrochemical performances was made. The edge plane of MoS_2 crystal showed a significantly higher electrochemical activity than the basal plane.

Our calculations are performed by means of density functional theory (DFT) implemented in program package GPAW. These calculations yield detailed information on the electronic and atomic structure, properties of MoS_2 surface cuts, properties in the bulk and its complexes with transition metals. We have determined the most energetically preferable surface cuts of MoS_2. Structure optimization between the surface of MoS_2 and Au with varied thickness was carried out. The tendency of gold to attach to the ideal edge surface of MoS_2 layers and forming a contact was observed.

[1] A. Splendiani, L. Sun, Y. Zhang, T. Li, J. Kim, C.-Y. Chim, G. Galli, F. Wang, Nano Lett. 2010, 10, 1271–1275.
[2] H. Liu, A. T. Neal, and P. D. Ye, ACS Nano 6, 8563 (2012).
[3] J. Kang, W. Liu, D. Sarkar, D. Jena, K. Banerjee, Phys. Rev. X 2014, 4, 031005.
[4] S. M. Tan, A. Ambrosi, Z. Sofer, Š. Huber, D. Sedmidubský and M. Pumera, Chem. – Eur. J., 2015, 21, 7170–7178.