Theoretical exploration of two-dimensional electrenes for low-resistance metal-2D semiconductor contacts

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Transition-metal dichalcogenides (TMDCs), including MoS_2, have great potential in electronic applications. However, achieving low-resistance metal contacts is a challenge that impacts their performance in nanodevices, due to strong Fermi-level pinning and the presence of a tunnelling barrier. As a solution, we explore a strategy utilizing two-dimensional (2D) alkaline-earth sub-pnictide electrenes with a general formula of M_2X (M = Ca, Sr, Ba; X = N, P, As, Sb) as an intermediate material between the 2D TMDC and metal. Electrenes possess one excess electron per formula unit resulting in the formation of 2D sheets of charge on their surfaces. This charge can be readily donated when interfaced with a TMDC semiconductor, thereby lowering its conduction band below the Fermi level and eliminating Schottky and tunnelling barriers. Density-functional theory calculations were performed on metal-electrene-MoS_2 heterojunctions for all stable M_2X electrenes, and both Cu and Au metals. To identify the material combinations that provide the most effective Ohmic contact, the charge transfer, band structure and electrostatic potential, among other quantities, were analyzed. A linear correlation was found between the charge donated to the MoS_2 and the electrene surface charge. Ca_2N is found to be most promising for achieving an Ohmic contact, due to its high surface charge density. Next, we performed electronic structure calculations for Cu/Ca_2N/TMDC interfaces (TMDC = $MoSe_2$, $MoTe_2$, WS_2 and WSe_2). The electrene insertion strategy is found to be effective for creating Ohmic metal contacts with other 2D TMDCs.

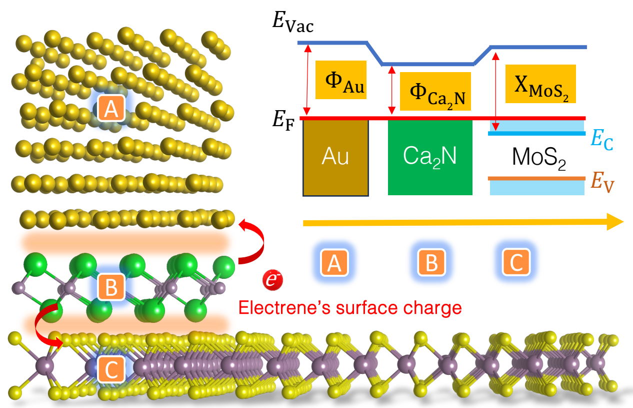

Fig. 1. Schematic design of the Au/MoS_2 interface with monolayer Ca_2N as an intermediate layer. The associated band diagram indicates the removal of the Schottky barrier upon metallization of the MoS_2 bands.