Currently, semiconducting layered sulfide nanostructures of MoS$_2$ and WS$_2$ are considered as possible alternatives for graphene in electronic devices. The structure of these materials results in a highly inert surface with a low defect concentration, which enable the fabrication of FETs with an intrinsically low field-effect threshold and a high mobility of charge carriers. Consequently, the fabrication of a FET based on single layered MoS$_2$ has been demonstrated recently.[1]

In order to understand the nature of MoS$_2$/metal contacts, we performed ab initio density functional theory calculations for the geometry, bonding and electronic structure of the contact region. We have also studied the I-V characteristics of a device as described in [1], using a Drift-Diffusion model and demonstrate the capabilities of such devices.