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# Ab Initio Simulations of Defective Metal Contacts in Beyond-CMOS Devices Based on Single-layer MoS<sub>2</sub>: Impact of Small and Extended Defects

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Atomically thin single-layer molybdenum disulfide (MoS<sub>2</sub>) is a two-dimensional material with highly desirable mechanical, electronic, and optical properties. These, combined with its reduced dimensionality and ultra-thin size, could enable the fabrication of a new generation of very compact and low-power devices which go beyond the conventional CMOS technology.

At present, wafer-scale production of MoS<sub>2</sub> is mainly achieved via CVD and PVD growth techniques, however, films have not yet reached the level of purity typical of the silicon technology. Small and extended defects are inevitably introduced in the material, and are expected to significantly affect not just the properties of MoS<sub>2</sub> itself but also the quality of the metal contact. For instance, poor electron injection and Fermi level pinning at the MoS<sub>2</sub>-metal interface could lead to large Schottky barriers and contact resistances, which limit the device performance by introducing unwanted parasitic elements [1]. This is detrimental for devices like field-effect transistors (FETs). On the other hand, the functionality of some devices, such as memristors based on monolayer MoS<sub>2</sub>, may even depend on the presence and nature of such defects [2].

Here, with the aim of bridging the gap between material's properties and device physics, we investigate defective single-layer MoS<sub>2</sub> in top contact with a metal electrode. To do so, we carry out ab initio computer simulations in the framework of Density Functional Theory (DFT) coupled with surface simulations based on the Green's function formalism [3]. Such a simulation scheme allows us to construct realistic MoS<sub>2</sub>-metal interfaces and to carry out accurate interface simulations. To model the metal electrode, we choose the chemical inert Au as it is commonly employed at the lab scale to fabricate devices. We explore the impact of experimentally-observed vacancies and substitutions on the properties of MoS<sub>2</sub>-Au contacts, and we predict relevant interface properties such as electron injection rates and tunnelling barriers.

Ultimately, our study constitutes the first step of a more comprehensive multi-scale modelling approach, in which the aim is to construct a full atomistic-to-device level model that can aid us in elucidating the physics of 2D devices based on single-layer MoS<sub>2</sub>.

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## References

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