# MECHANICAL BEHAVIOUR OF $MoS_2$ NANOSHEETS UNDER STRESS AND ASSOCIATED FUNCTIONAL PROPERTIES

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*3-year contract*: 1768 € raw monthly salary

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**Framework and objectives.**
Many international researches are now oriented toward 2D materials that present the interest of an ultimate thickness of only a few atomic layers. Among them, Transition Metal Dichalcogenide (TMDC) combine a graphene-like 2D morphology with semiconductive functionnal properties[1]. They offer new ways for technological challenges in various domains[2,3] like microelectronics, photovoltaic or catalytic chemistry. In addition, the development of flexible devices requires a high mechanical stability under severe operating conditions. Understanding how 2D materials will respond to external applied stresses and how the morphological changes may modify, or even control, their functional properties appears consequently of primary importance in a near future.
The scientific approach recently developed at the Pprime institute (University of Poitiers, France) consists in monitoring by UHV AFM/STM the in situ evolution of surface, down to the atomic scale, at increasing stress or strain (Nanoplast equipment[4]). In particular, it allows controlling deformations on crystalline substrates and hence locally modifying the morphology of the covering thin films or foils in interaction.

**Work program and means.**
This PhD work will be focused on molybdenum disulfur ($MoS_2$) of the dicalcogenur family exhibiting semiconductor properties. The elementary sheets consist of only 3 atomic layers and present the advantage to be compatible with flexible transparent substrates[5]. The aim is to have a better understanding of their mechanical behavior under stress and to identify how their catalytic or electronic properties may be modified or enhanced.
This PhD proposal will combine experimental and theorical work. The experimental part includes the transfer of $MoS_2$ nanosheets from their growth substrate to single crystalline substrates of interest like Au or Cu[6]. Their observation will then be carried out by local

probe microscopies (STM and non-contact AFM). The role of key-parameters (such as substrate materials, adhesion properties, structure and thickness of the foil, deformation temperature) will be studied. Finally, atomistic simulations using interaction potentials (for mechanical behavior) and/or DFT ab initio calculations (for electronic band structures) will be considered (collaboration with CEA-Saclay, France).

**Applicant profile, prerequisites.**

Masters, Diploma or equivalent degree in Physics or Physical Chemistry.
Strong background and interest in material science, especially in surface science and plasticity.
Experience with SPM techniques (STM or AFM), preferencially under UHV, and Background in physical behavior of layered materials would be appreciated.

**Application deadline : 15 april 2019**

**Bibliography.**

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