


**Internship proposal 2009-2010**

<p><b>Laboratory :</b> Institut de Minéralogie et de Physique des Milieux Condensés</p> <p><b>Address :</b> 140 rue de Lourmel, 75015 Paris (Campus Boucicaut)</p> <p><b>Laboratory director :</b> Bernard Capelle</p>	
<p><b>Internship supervisor :</b> Matteo Calandra</p> <p><b>Phone :</b> 01 44 27 52 16</p> <p><b>e-mail:</b> matteo.calandra@impmc.jussieu.fr</p> <p><b>web-page:</b> http://www.impmc.upmc.fr/~calandra/</p>	

**FLEXIBLE ELECTRONICS AT THE NANOSCALE**

Recently, several nanodevices based on single-layer transition-metal-dichalcogenides ( $\text{NbSe}_2$ ,  $\text{TaS}_2$ ,  $\text{TaSe}_2$ ...) were developed. These devices have many advantages respect to standard  $\text{SiO}_2$  field effect transistors (FET) as they have fairly high mobility and low field-effect threshold, they can operate both in electron or hole doped mode and, last but not least, they can be used as flexible nanoelectronic devices since when mounted on parylene gate dielectric they survive bending better than

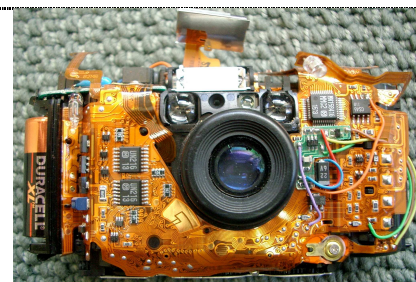


Fig. 1: Modern digital camera showing flexible electronic circuits

organic-based FET which are the basis of flexible electronics. Nowadays flexible circuits are used in applications where flexibility and space savings limit the serviceability of rigid circuits. Prominent examples are cameras or the switch matrix of computer keyboards (see fig. 1). Despite the big experimental efforts, the behaviour of single-layer transition metal dichalcogenides in a field-effect transistor, as a function of the applied electric field is largely unexplained. Surprisingly, and contrary to what one would expect from the metallic behaviour of the bulk  $\text{NbSe}_2$ , the conductivity of a  $\text{NbSe}_2$  single-layer in a FET shows a strong monotonic dependence on the gate voltage, (a variation of more than a factor of two in the -70 to +70 V range), similar to what happens in Graphene. The explanation of this surprising behaviour was recently given by our theoretical group (M. Calandra *et al.* [arXiv:0910.0956](https://arxiv.org/abs/0910.0956)). We have demonstrated that single-layer  $\text{NbSe}_2$  undergoes a charge-density wave instability generated by the interaction between the electrons and the lattice vibrations. The system becomes then unstable towards a semimetallic state, contrary to what happens in the bulk where the charge density wave leaves the system metallic. The correspondent conductivity is much more similar to that of an insulator than to that of a metal, in agreement with experimental data. This work is a first necessary step for the understanding of transition-metal-dichalcogenides nanodevices, but there are still several unknown issues. What happens to other single-layer transition-metal-dichalcogenides ( $\text{TaS}_2$ ,  $\text{TaSe}_2$ ) ? And what about insulating dichalcogenides such as  $\text{MoS}_2$ , that have never been studied from the theoretical point of view ? What are generally the properties of their associated single-layers ? The ultimate goal of the internship is to answer these questions, an important step for the development of flexible nanoelectronics.

**Techniques in use :** Theoretical methods (mainly numerical) including density-functional-theory and state-of-the-art numerical simulation in general.

**Applicant skills :** Good background in quantum mechanics and solid state physics in general

**Granted internship :** yes  
**C'nano IdF laboratory (France only) :** yes  
**Possibility for a thesis :** yes (type of grant : ministry of research)