Native Cesium Doping and Metal Insulator Transition in a MoS$_2$ Nanosheet.

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MoS$_2$ is one of the most attractive emerging research materials for nanotechnology [1],[2]. As belonging to the class of layered transition metal dichalcogenides (TMDs), it can be reduced to a stable single layer by tuning its semiconducting character from an indirect to direct band-gap [3]. This makes it complementary to graphene in terms of applications to nanoelectronics where the presence of a bandgap allows for an effective charge commutation and hence for logic operation and optoelectronic activity [4]. These features along with the intrinsic n-type carrier transport have made MoS$_2$ nanosheets as outstanding candidates to engineer ultimately scaled field effect transistor with promising perspectives for the next technological nodes in the semiconductor roadmap [5].

In the present work, we elucidate this aspect by examining the chemical composition of rheological MoS$_2$ multilayer nanosheets mechanically exfoliated on SiO$_2$/Si substrates by making evidence of the native incorporation of cesium atoms in the MoS$_2$ crystal. Since Cs belongs to the alkali metals, the incorporation of Cs atoms in the MoS$_2$ layered structure may effectively act as an electron donor dopant upon activation of a charge exchange with the conduction band of the MoS$_2$. Cs doping of MoS$_2$ nanosheets is assessed by energy dispersed X-ray spectroscopy (SEM-EDX) and secondary ion mass spectroscopy (SIMS). In addition electrically detected magnetic resonance (EDMR) spectroscopy of paramagnetic centers in a MoS$_2$ crystal is carried out to evaluate the electrical activity of the Cs dopant atoms. EDMR reveals an anisotropic signal related to a Cs impurity and two other smaller signals associated with S and Mo vacancies. This effect is supported by ab-initio calculations and experimental evidences thereby clarifying the n-type character of commercially supplied MoS$_2$ crystals.

From an extensive compositional analysis of natural MoS$_2$ crystals we show that Cs impurities are incorporated to an amount of 1% throughout the whole MoS$_2$ crystal. Based on ab initio calculations, Cs atoms can be stabilized in the MoS$_2$ when intercalated in between MoS$_2$ planes and in concentration of 1% they prove to generate a doping level in proximity of the MoS$_2$ conduction band edge. Not only this intrinsic doping confers the well-know n-type character to the MoS$_2$, but also Cs impurities are associated with an increase the carrier concentration inside the MoS$_2$ multilayer field effect transistor In this respect, the native Cs atoms effectively behave as a doping species which, in certain range of gate bias and forward in-channel field, drag the MoS$_2$ from an insulating state to a metallic one as inferred from the temperature dependent electrical transport in a MoS$_2$ multilayer nanosheet field effect transistor (FET).

References