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 dichalchogenides (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 SiO2/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 MoS2 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 MoS2, but also Cs impurities are associated with an increase the carrier concentration inside the MoS2 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 MoS2 from an insulating state to a metallic one as inferred from the temperature dependent electrical transport in a MoS2 multilayer nanosheet field effect transistor (FET).

References

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