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Structures, electronic and magnetic properties of transition metal doped MoS2 intercalation compounds[1] HONG-DAO LI, TAI-SING WU, HORNG-TAY JENG, Department of Physics, National Tsing Hua University, Taiwan, SHIH-LIN CHANG, National Synchrotron Radiation Research Center, Taiwan, YUN-LIANG SOO, Department of Physics, National Tsing Hua University, Taiwan — Molybdenum disulfide (MoS2) has recently attracted much attention due to its potential applications in high efficiency hydrogen storage, catalysts, and nanoelectronic devices. While intrinsic MoS2 bulk is a well-known diamagnetic material, zigzag nanoribbons of MoS2 have been predicted by density functional theory (DFT) to be metallic and ferromagnetic. The effects of transition metal (TM) doping on the magnetic properties of MoS2 appear to be a very interesting issue. In this work, we have synthesized a series of TM (Co,Ni,Cu) doped MoS2 intercalation compounds by an exfoliation/restacking method with different TM concentration (0.01-10 at. %) and annealed at various temperatures (300-1000K). Raman spectra and x-ray diffraction (XRD) data show that the synthesized TM-MoS2 intercalation compounds are in 2H-MoS2 structure with average size ∼100 nm. The average distance between MoS2 host layers strongly depends on the TM concentration. XANES and EXAFS reveal that TM atoms are located on tetrahedral sites between the MoS2 sheets with valence number +1. A series of DFT simulations indicate that Co-MoS2 may exhibit half-metallic ferromagnetic states while ferromagnetism is absent in Cu-MoS2 and Ni-MoS2. Experimental data obtained from magnetic measurements will also be presented.

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