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Magnetization and magnetic anisotropy of 3d adatoms on a MoS_2 monolayer[1] MARCIO COSTA, JUN HU, RUQIAN WU, Univ of California - Irvine — MoS_2 is layered semiconductor that goes under a transition from indirect (bulk - 1.2 eV) to a direct (monolayer - 1.8 eV) gap. MoS_2 monolayer has been drawing attention due to its peculiar transport properties, with mobilities of 200 cm^2 V^{-1} s^{-1} at room temperature. Using Density Functional Calculations, we studied the adsorption of transition metal adatoms on the MoS_2 monolayer. The adsorption energies of Mn, Fe, Co and Ni on MoS2 monolayer were calculated over different sites. We also determined their magneto crystalline anisotropy (MCA) energies, for the purpose of using these systems in spintronic devices. To manipulate the magnetic properties, the effect of coadsorption of Bi and other elements were also investigated.

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Jun Hu
Univ of California - Irvine

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