Itinerant ferromagnetism in p-doped monolayer of MoS_2

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Abstract

We use density functional theory to explore the possibility of making the semiconducting transition metal dichalcogenide MoS_2 ferromagnetic by introducing holes into the narrow Mo 4d band that forms the top of the valence band. In the single impurity limit these hole bound-states polarize completely. Pairs of holes couple ferromagnetically for all but the shortest separations when the bonding interaction makes it energetically favourable to form spin singlets. Using the calculated separation dependent ferromagnetic exchange interaction between pairs of these moments in dilute $Mo_{1-x}V_xS_2$ random alloys as input to Monte Carlo calculations[1], we estimate ordering temperatures as a function of x. For x ~ 9%, Curie temperatures in excess of 160 K for V doping are predicted. Suggestions are made to increase this above room temperature.

References

[1] K. Binder, Z. phys. B, 43, (1981) 119-140

Figures

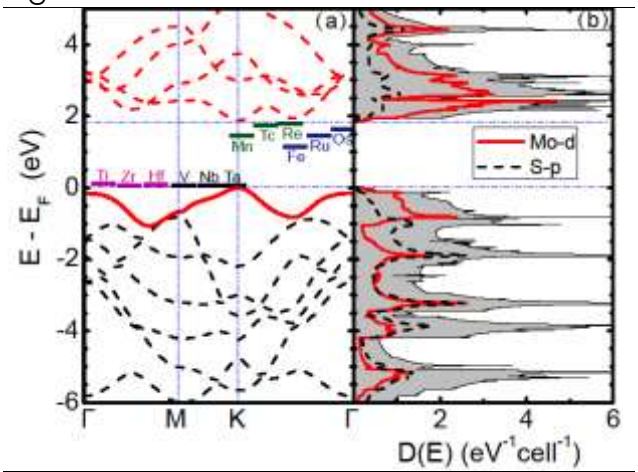

Figure 1: The band structure and density of states of an MoS_2 monolayer. (various substitutional defect levels are indicated).

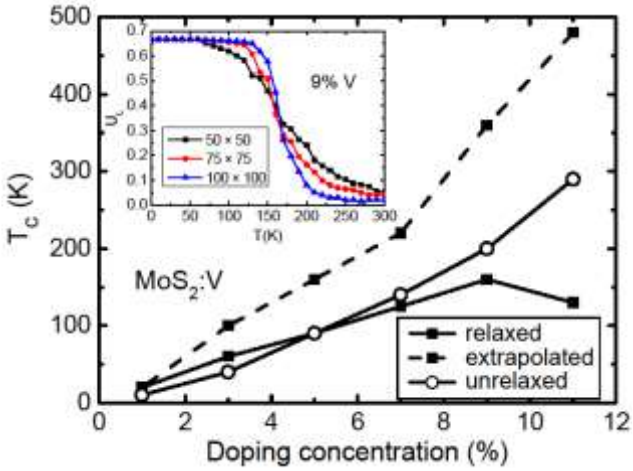

Figure 2: Variation of the ferromagnetic Curie temperature as a function of the doping concentration for an MoS_2 monolayer doped with V. The dashed curve was calculated by extrapolating the relaxed exchange interactions to separations where quenching occurs.