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Structural, electronic, and magnetic properties of transition metal doped ReS_2 monolayer

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Two-dimensional (2D) nanosheets have been wildly studied due to their exotic physics and potential applications in nanoelectric devices. Typically, graphene and MoS_2 have gained much interest. Similar to MoS_2, a new 2D TMD, ReS_2, has been fabricated and received a lot of attentions. As is well known, transition-metal (TM) atoms could induce magnetism, scattering and superconduction at a low doping concentration and modify the electronic structure obviously. It may exhibit novel and intriguing properties for studying TM atoms doped ReS2 monolayer. Thus, we systematically examine the structural, electronic, and magnetic properties of ReS_2 monolayer doping with different TM (TM = Co, Cu, Mn, Fe, and Ni) atoms, as shown in Fig. 1a.

Magnetism is observed in the cases of Co, Fe, and Ni. Among three magnetic cases, the Co-doped system shows a largest magnetic moment. Therefore, the interaction between two-Co-doped ReS_2 monolayer is further studied, and several possible configurations of Co dopants are shown in Fig. 1b. A ferromagnetic (FM) coupling induced by the $p-d$ hybridization between Co and S atoms is observed. However, the FM coupling is obviously depressed by the increasing Co–Co distance, which can be well described using a simple Heisenberg model based on Zener theory (Fig. 1c). Such interesting phenomena might be suitable for potential applications in electronics and spintronics. Our full text of the article will be published in the "JETP Letters" journal.

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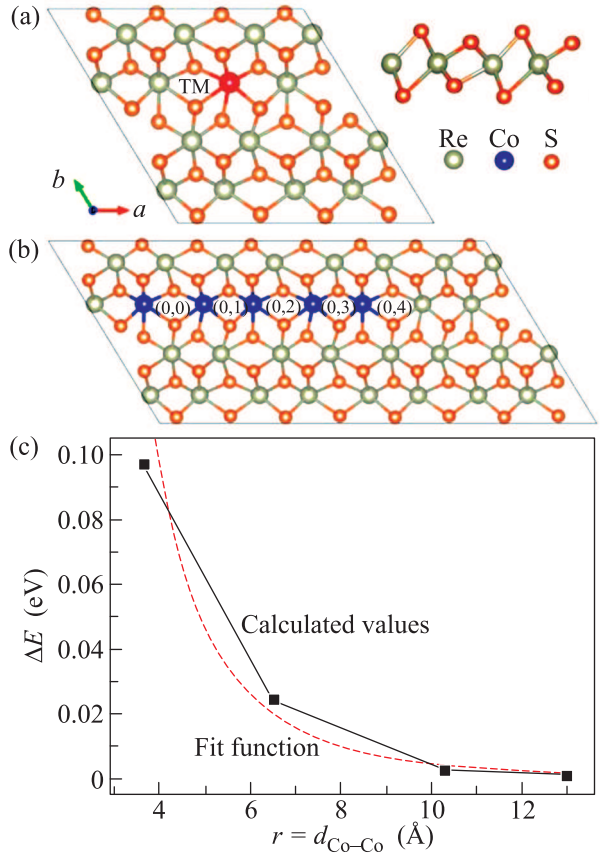

Fig. 1. (Color online) (a) – Top and side view of one TM-doped ReS_2 monolayer of $2\times2\times1$ supercell; (b) – the configurations in two-Co-doped ReS_2 monolayer of $4\times2\times1$ supercell; (c) – the total energy difference (ΔE) as a function of the Co–Co distance (r), $r = d_{\text{Co-Co}}$. The dashed line is the magnetic correlation function $J(r)$ vs the Co–Co distance (r) $\Delta E = E_{\text{AFM}} - E_{\text{FM}}$

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