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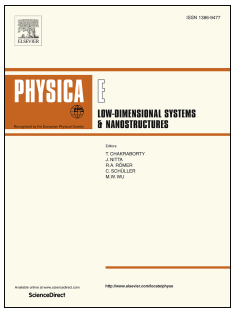

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Ferromagnetism in monolayer MoS_2 dictated by hydrogen adsorption sites and concentration

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Abstract

We show that hydrogen-induced magnetism in monolayer MoS_2 is dictated by the hydrogen adsorption sites and concentration by using density functional theory calculations. Hydrogen adsorbed at the center of the hexagonal ring leads to an itinerant ferromagnetism at relatively high concentrations, whereas hydrogen adsorbed on sulfur leads to a flat-band ferromagnetism at a relatively low concentration. The electrons in the non-metallic flat-band ferromagnetism are equally distributed on hydrogen and nearby Mo and S atoms, in contrast to the non-magnetic case where they are concentrated on the nearby Mo atoms.

Key words: Monolayer MoS_2; Hydrogen adsorption; Ferromagnetism; DFT calculations

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