Magnetic adatoms on two-dimensional $NbSe_2$

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In the last decade, much research has been focused on quasi-two-dimensional magnetism in monolayers or buried interfaces [1]. Two-dimensional transition metal dichalcogenides are very interesting from a fundamental point of view, as magnetism and charge-density waves compete with each other. Magnetic impurities may modify a charge-density wave, by altering its energetic stability as well as its local patterns. The charge density wave in turn affects how magnetic impurities can interact with each other, modulating the exchange coupling. Therefore, inducing magnetism with external chemical species has the potential to be an effective way to engineer new electronic and magnetic phases in perspective of technological applications. In this poster, we present our study on the extrinsic magnetism arising from adsorbed transition metals on two-dimensional $NbSe_2$ [2,3]. We demonstate that each investigated adatom (Cr, Mn, Fe, and Co) can be located in various metastable positions on the monolayer, inducing substantial modifications in the local patterns of the charge densities [2]. The coupling between magnetic impurities is then investigated by means of the magnetic force theorem [3]. Our results show that the exchange coupling has an oscillatory nature accompanied by an exponential decay, typical of a damped RKKY interaction [4]. The oscillatory behavior can be traced back to a single nesting vector in the Fermi surface, which is not affected by small changes on the height of the impurity, making magnetism robust against external perturbations.

References:

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