Magnetic skyrmions of Ti2C MXenes doped with Cr, Mn, and Fe

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Two-dimensional titanium carbides Ti2C, MXenes, have been attracted scientific effort, mostly owing to their intriguing properties and promising applications [1]. The magnetic moments of the external metallic Ti layers are ferromagnetically or antiferromagnetically oriented to each other depending on the remnants from the technological processes that cover the surface. The possibility to tune magnetic moments of the external MXenes layers through suitable functionalization could be utilized in numerous spintronic applications [2].

We have investigated the change of the magnetic properties of MXenes caused by the substitutional doping of Ti layers with transition metal (TM) atoms such as Mn, Cr, and Fe. The introduction of TM atoms with different numbers of d-electrons (and therefore different magnetic moment) leads to breaking of the homogeneity of the spontaneous magnetization and formation of the skyrmionic-like patterns. Magnetic skyrmions are small swirling topological defects in the magnetization texture, which are regarded as novel information carriers in future spintronic devices [3].

Our studies are based on the first principles calculations within the Kohn-Sham realization of the density functional theory (DFT) employing the Quantum Espresso computer package. We take spin-orbit interaction into account, and therefore, our calculations have to be performed in the non-collinear magnetism regime. To facilitate eventual future comparison with experiments, we have undertaken an attempt to compute the spin tunneling current between the non-uniformly spin-polarized electrons of the MXenes surface and magnetic tip of the scanning tunneling microscope (STM), in close analogy to codes providing the STM images from the electronic density obtained in DFT calculations.

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