

# Theoretical prediction of two-dimensional magnetic materials

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## Abstract

Using first-principles calculations, we show some interesting magnetic behaviors in two-dimensional atomic crystals. For pristine atomic crystals, it is difficult to get ordered spin structures. In our research, we will show that organic porous sheet has important magnetic behaviors, and demonstrate the existence of half-metallicity. Moreover, we will show that the ultrathin films of recently experimentally realized wurtzite MnO transform into a stable graphitic structure with ordered spin arrangement and the stability of graphitic structure can be enhanced by external strain. Furthermore, we found the antiferromagnetic ordering of graphitic MnO single layer can be switched into half-metallic ferromagnetism by slightly doping.