# First-principles study of two-dimensional transition metal carbides (MXenes)

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## ABSTRACT

MXenes are a new family of two dimensional early transition metal carbides recently synthesized by extraction of the "A" layers from the MAX phases. Using first-principles calculations, we have studied the mechanic and magnetic properties of MXenes. Firstly, we show that the mechanical failure of MXene under tensile strain is due to the elastic instability induced by the rapid collapse of the surface metal layer. When the MXene surfaces are functionalized by F, OH, or O groups, this collapse under strain slows down, resulting in the striking increase in the ideal strength of MXene. Secondly, we identified a half metallic ferromagnet among the family of MXenes, i.e., $Cr_2C$ MXene, which has a half-metallic gap of 2.85 eV, large enough for the room temperature operation. $Cr_2C$ MXene also shows a ferromagnetic (FM) to antiferrmagnetic (AFM) phase transition induced by the surface functionalization. The FM to AFM transition is accompanied by a metal to insulator (MIT) transition, with the energy gap in the antiferromagnetic insulating state controllable by changing the type of the functional groups. Finally, we further reveal that the underlying mechanism for the FM-AFM and MIT transition, which is the localization of Cr *d* electrons induced by the surface functionalization. Our results demonstrate the potential applications of MXenes in flexible electronics and spintronics.