Biocompatible Ferromagnetic Cr-Trihalide Monolayers QIANG SUN, Peking University — Cr with an electronic configuration of 3d^54s^1 possesses the largest atomic magnetic moment (6\(B\)) of all elements in the 3d transition metal series. Furthermore, the trivalent chromium (Cr\(^{3+}\)) is biocompatible and is widely found in food and supplements. Here using first principles calculations combined with Monte Carlo simulations based on Ising model, we systematically study a class of 2D ferromagnetic monolayers CrX\(_3\) (X= Cl, Br, I). The feasibility of exfoliation from their layered bulk phase is confirmed by the small cleavage energy and high in-plane stiffness. Spin-polarized calculations, combined with self consistently determined Hubbard U that accounts for strong correlation energy, demonstrate that CrX\(_3\) (X=Cl, Br, I) monolayers are ferromagnetic and Cr is trivalent and carries a magnetic moment of 3\(B\), the resulting Cr\(^{3+}\) ions are biocompatible. The corresponding Curie temperatures for CrCl\(_3\) CrBr\(_3\) CrI\(_3\) are are found to 66, 86, and 107 K, respectively, which can be increased to 323, 314, 293 K by hole doping. The biocompatibility and ferromagnetism render these Cr-containing trichalcogenide monolayers unique for applications.

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