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Biocompatible Ferromagnetic Cr-Trihalide Monolayers QIANG SUN, Peking University — Cr with an electronic configuration of $3d^5 4s^1$ 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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