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High Temperature Ferromagnetism in π-Conjugated 2D Metal-Organic Frameworks[1] WENBIN LI, LEI SUN, JINGSHAN QI, PABLO JARRILO-HERRERO, MIRCEA DINCA, JU LI, Massachusetts Institute of Technology — We use first-principles calculations to design a new class of phthalocyanine (Pc) based 2D metal organic frameworks (MOFs) with square lattices that exhibit rich magnetic behavior. A MOF made from MnPc connected through Ni-bisphenylene-diimine moieties, NiMnPc, was found to exhibit a ferromagnetic ground state with a large exchange energy, resulting from the unique strong hybridization between the d/π orbitals of Mn, the Pc ring, and the Ni nodes. Notably, we show that for NiMnPc there is a considerable difference between the ferromagnetic ordering temperature (T_c) predicted by a 2D Ising model, which exceeds 600 K, and a T_c of 170 K predicted by our more realistic Monte Carlo simulation that includes magnetic anisotropy. In the bulk, 2D layers of NiMnPc adopt a slipped-parallel stacking configuration, and exhibit interlayer magnetic coupling that is sensitive to the relative in-plane displacement between adjacent layers. The results highlight the critical role of magnetic anisotropy in modeling the properties of 2D magnetic systems. More generally, it demonstrates that strong hybridization between open-shell ions and delocalized aromatic π systems, combined with large magnetic anisotropy, will be an effective design strategy to realize ferromagnetic 2D MOFs with high T_c.

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