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First-Principles Design of a Half-Filled Flat Band of the Kagome Lattice in Two-Dimensional Metal-Organic Frameworks MASAHIKO G. YAMADA, Institute for Solid State Physics, University of Tokyo, TOMOHIRO SOEJIMA, Department of Chemistry, Massachusetts Institute of Technology, NAOTO TSUJI, RIKEN Center for Emergent Matter Science (CEMS), DAISUKE HIRAI, Department of Physics, University of Tokyo, MIRCEA DINCĂ, Department of Chemistry, Massachusetts Institute of Technology, HIDEO AOKI, Department of Physics, University of Tokyo — Metal-organic frameworks (MOFs) are crystalline materials composed of metal ions and bridging organic molecules, which have been the subject of numerous investigations in inorganic and materials chemistry. Owing to their typically trivial electronic states, MOFs have not attracted much attentions from condensed-matter physicists. However, recent experimental success in fabricating two-dimensional (2D) MOFs with kagome lattice structures is bridging the gap between condensed-matter physics and chemistry. Then, we design from first principles a new type of 2D MOFs with phenalenyl-based ligands to realize a half-filled flat band of the kagome lattice, which belongs to the lattice family that shows Lieb-Mielke-Tasaki's flat-band ferromagnetism. We find that *trans*-Au-THTAP(trihydroxytriaminophenalenyl) has an ideal band structure, where the Fermi energy is adjusted right at the nearly flat band. The spin-orbit coupling opens a band gap and gives a non-zero Chern number to the nearly flat band. This is a novel and realistic example of a system in which a nearly flat band is both ferromagnetic and topologically non-trivial. See arXiv:1510.00164.

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