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Intrinsic two-dimensional organic topological insulators in metal−dicyanoanthracene lattices.[1] LIZHI ZHANG, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112 — Based on the first-principles density functional theory calculations, we identify the two-dimensional organic topological insulator (OTI) states in Cu−dicyanoanthracene (DCA) lattice, a system that has been grown experimentally on Cu substrate. The freestanding Cu-DCA lattice presents the p_z-orbital Kagome bands with a Dirac point at the Fermi level. Our analysis, including analysis based on a tight-binding model, the calculated Chern numbers, and the semi-infinite Dirac edge states within the spin−orbit coupling gaps, confirms its intrinsic topological properties. The intrinsic TI states are found to originate from a proper number of electrons filling of the hybridized bands from Cu atomic and DCA molecular orbital based on which similar lattices containing noble metal atoms (Au and Cu) and those molecules with two CN groups (DCA and cyanogens) are all predicted to be intrinsic OTIs. Our findings facilitate the future experimental confirmation of intrinsic OTIs that requires no additional doping.

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