Supporting Information for

Transition-metal phthalocyanine monolayers as new Chern insulators

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Table 1S. The lattice constants, magnetic moments and exchange energy of TMPc.

	Fe	Mn	Mo	Ru	Ta	Re
a=b (Å)	10.680	10.707	10.717	10.773	10.807	10.791
M (μ_B)	2.0	3.0	4.0	2.0	1.0	3.0
E_{AFM}-E_{FM} (meV)	-27.1	51.9	6.1	56.2	-15.7	59.3

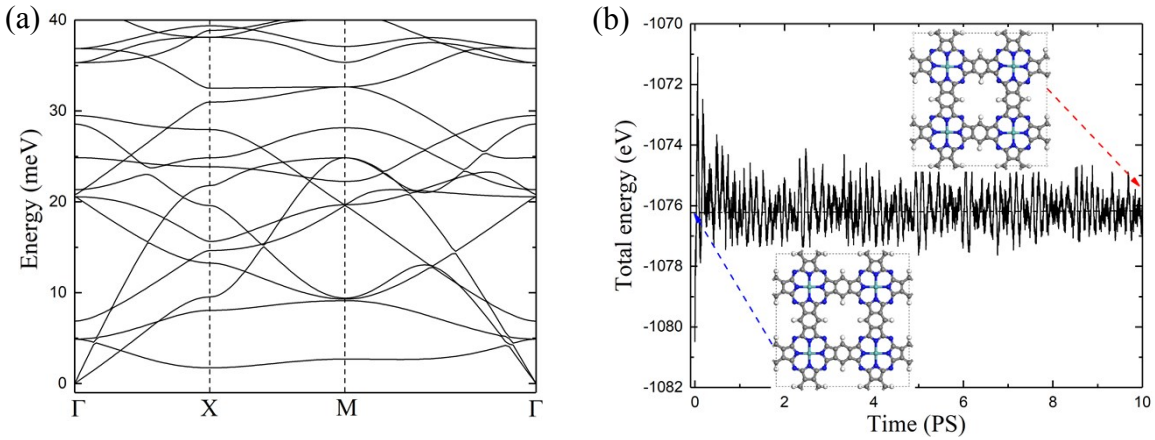

Fig. S1. (a)-(b) The phonon spectrum and the total energy as function of time for MoPc.

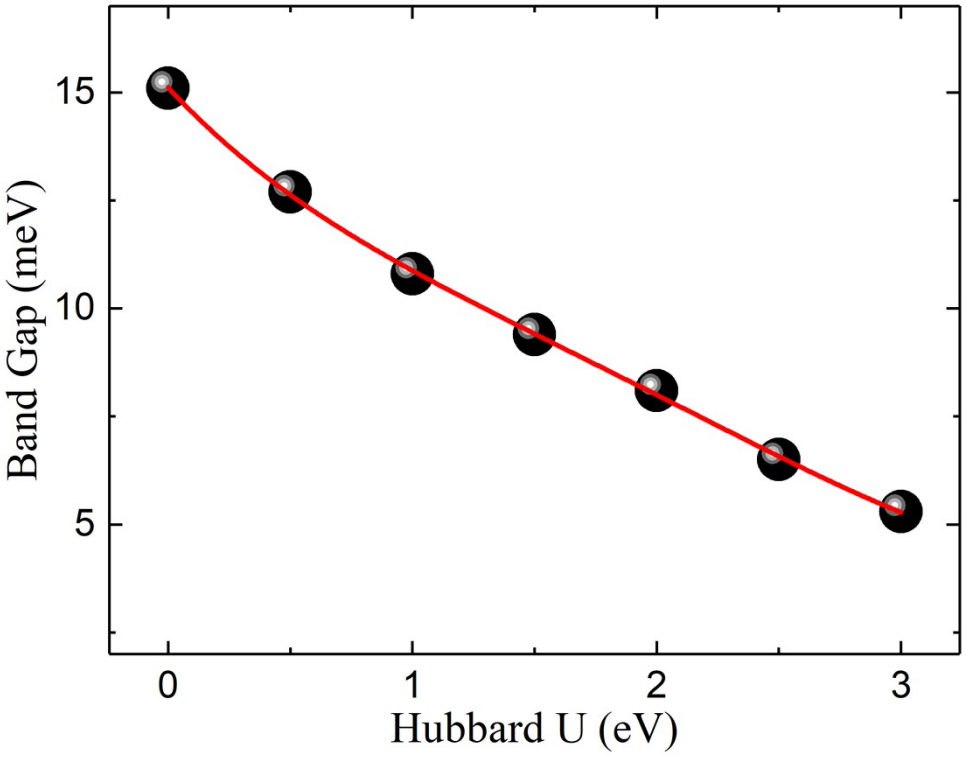

Fig. S2. The band gap as a function of Hubbard U for MoPc.

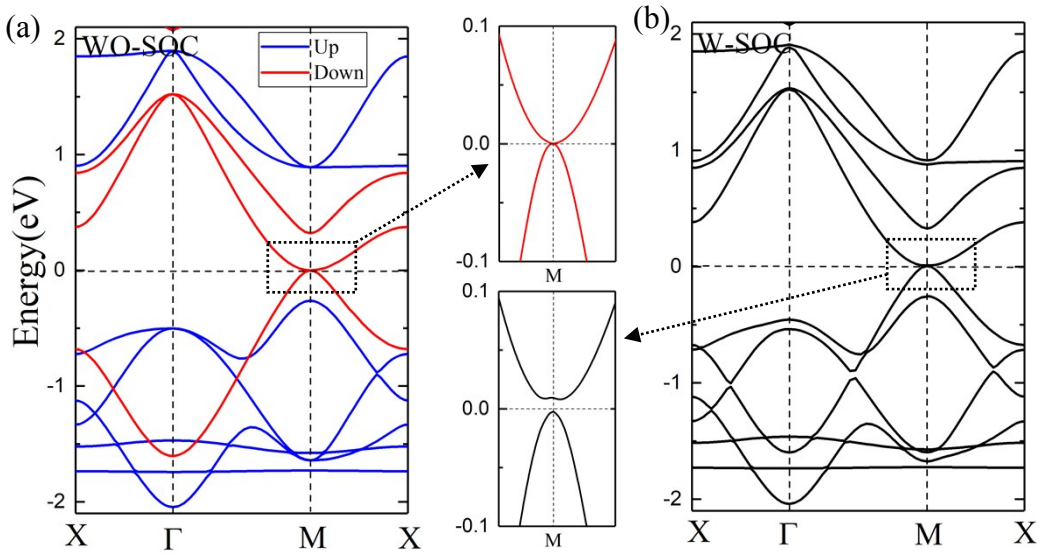

Fig. S3. (a)-(b) The band structure of MoPc without and with SOC by using the HSE06 calculations (the corresponding zoom-in band structures near the Fermi level around the M point are shown in the middle).

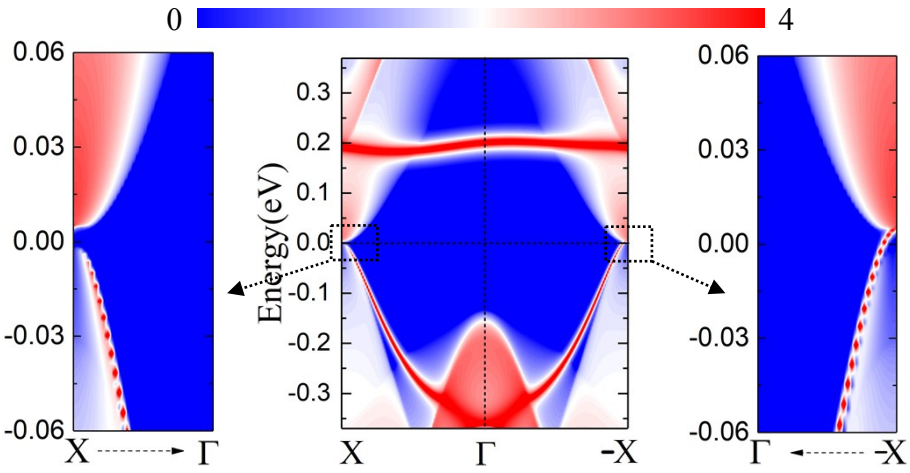

Fig. S4. The 1D band structure of the bottom edge of the MoPc ribbon.

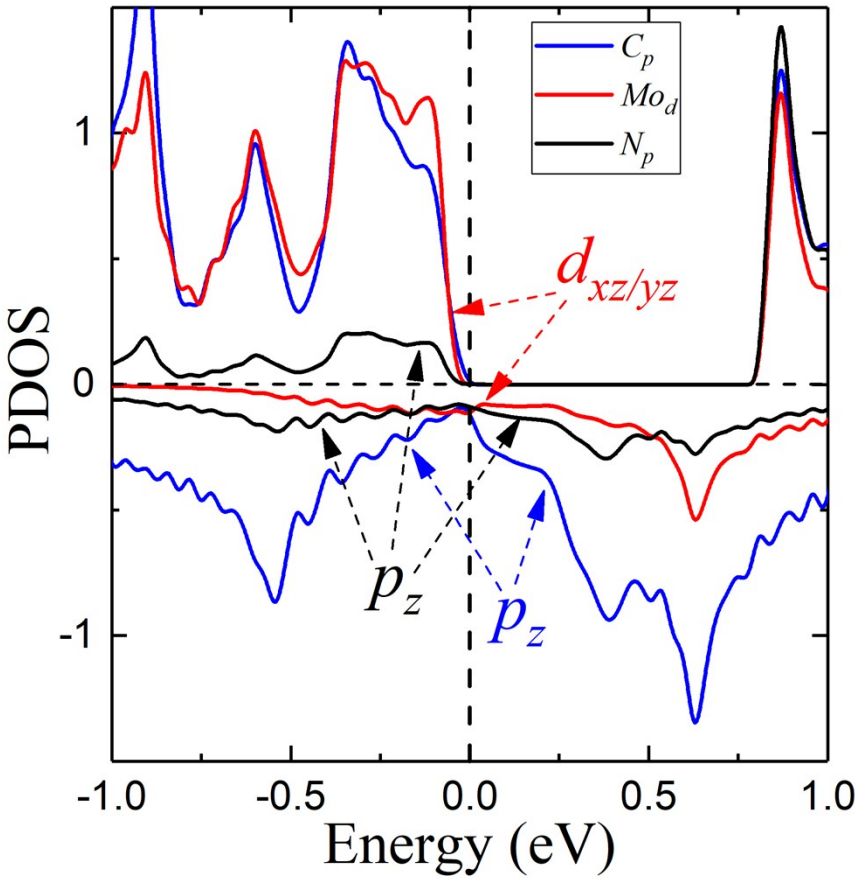

Fig. S5. The projected density of states of C, N and Mo atoms for MoPc.

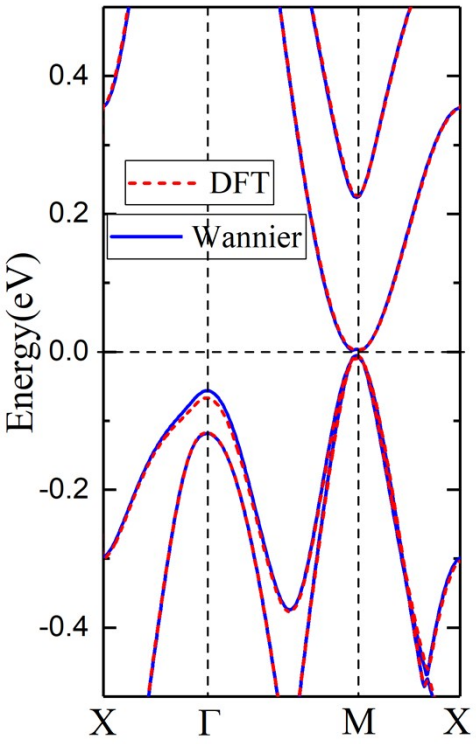

Fig. S6. The band structure of MoPc from DFT calculations and the fitting band structure by using Wannier90 package in which only the p_z orbitals of C and N atoms and $d_{xz/yz}$ orbitals of Mo atoms have been adopted as projected Wannier functions.

TB model detail:

Used parameters and their values for spin-up and spin-down channels are shown in figure S6(a) and (b), respectively. For orbitals at equivalent positions, only one hopping integral are denoted and others can be readily inferred from the wavefunction phases. For instance, for p_z orbitals symmetry about the vertical axis, their hopping integrals to the d_{xy} orbital are inverse numbers. Since spin-up and spin-down Hamiltonians are decoupled, we deal with the two spins separately. The parameter values are obtained by fitting the energy bands around the Fermi level. For the spin up bands, 2+1 (below and above the Fermi level, respectively) bands are used, and for the spin down bands, the setting is 1+2. For each band, X, Γ, M points are included in the sample data together with 7 points in every interval along the X-Γ-M-X path. The mean squared error is used for the optimization. For the spin-up channel, the lowest band is weighted by 0.5, so is the highest band for the spin-down channel.

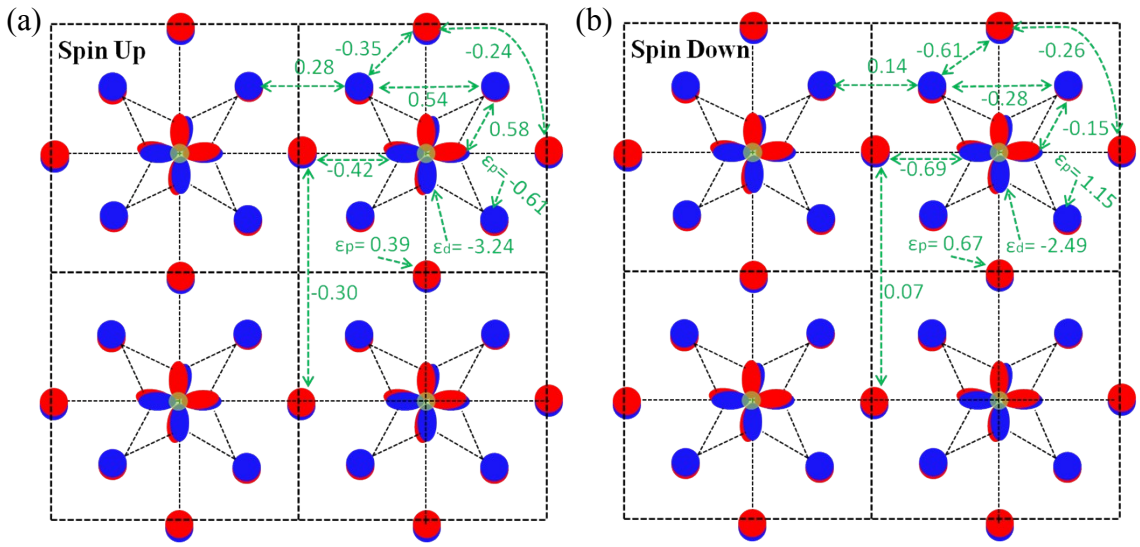

Fig. S7. (a) (b). Schematic spatial distributions of hopping integrals for spin up and spin down channels, respectively.

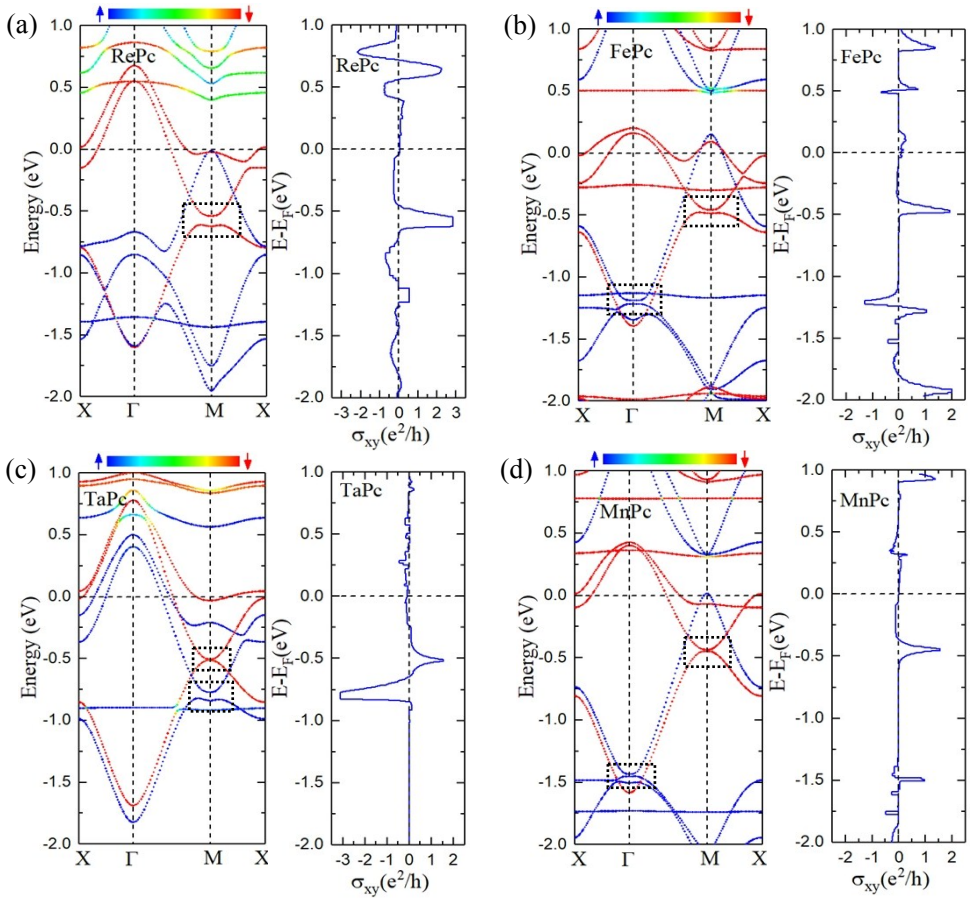

Fig. S8. (a)-(d) Band structures and corresponding Fermi level-dependent anomalous Hall conductance (σ_{xy}) for RePc, FePc, TaPc and MnPc, respectively. These nontrivial band gaps are shown in the dashed rectangle.