Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# SUPPLEMENTARY INFORMATION

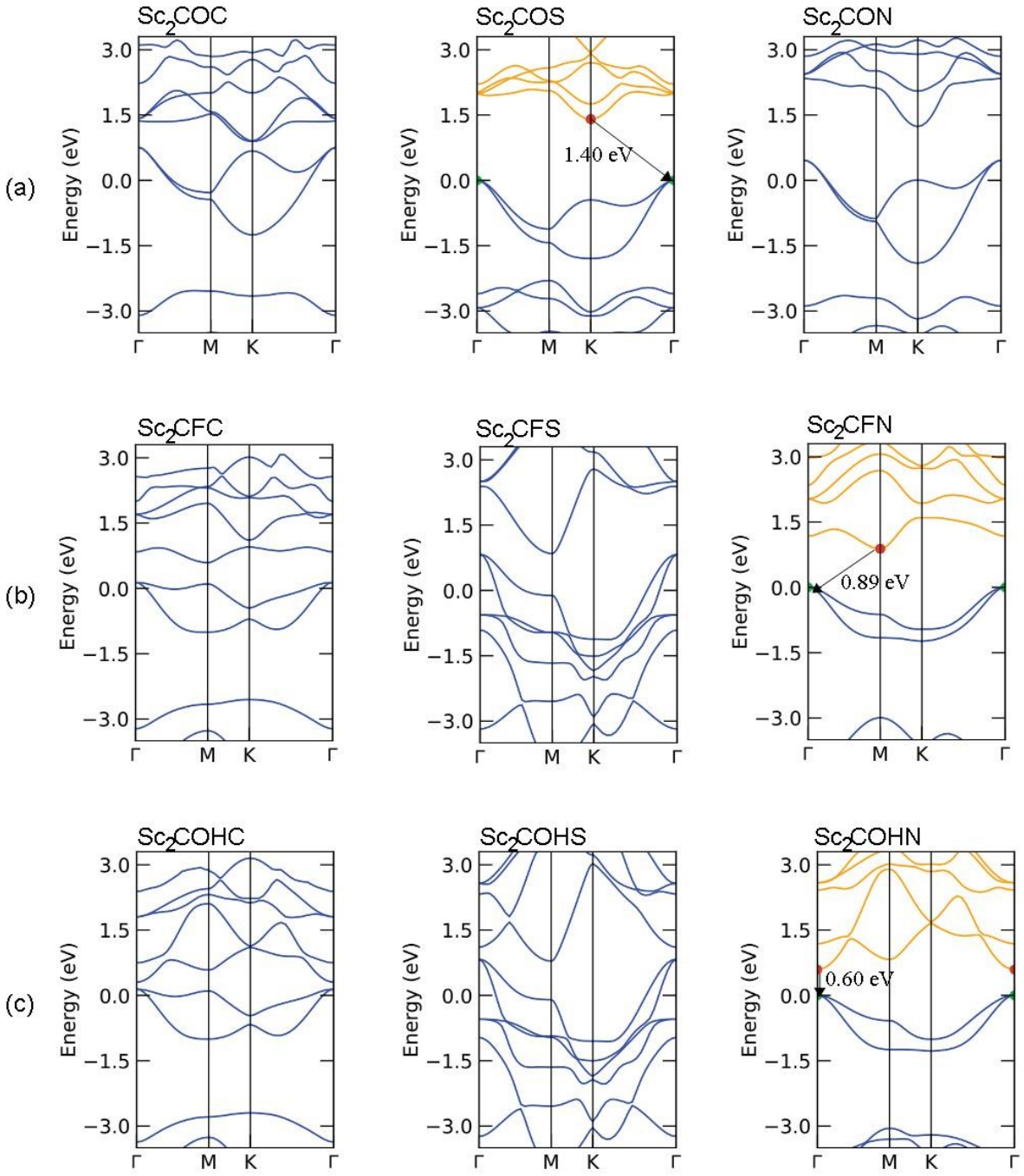


Fig S1. Band structures for the most stable models of (a) $Sc_2COT$, (b) $Sc_2CFT$, and (c) $Sc_2COHT$ monolayers (T= C, S, N). The Fermi energy is set at zero. Here, the band calculations are done without using the Heyd–Scuseria–Ernzerhof (HSE06) functional.

Table S1. The total energies (in eV) of non-magnetic ($E_{NM}$), ferromagnetic ($E_{FM}$), and antiferromagnetic ($E_{AFM1}$), ($E_{AFM2}$), and ($E_{AFM3}$) states (eV) for the most stable geometries of $Sc_2OC$, $Sc_2OS$, $Sc_2FS$, $Sc_2FN$, $Sc_2OHS$, $Sc_2OHN$, and $Sc_2CON$. The total magnetic moment values are zero for all the materials shown in Table S1 except for $Sc_2CON$.

| **Material** | **$E_{FM}$** | **$E_{NM}$** | **$E_{AFM1}$** | **$E_{AFM2}$** | **$E_{AFM3}$** | **Magnetic moment (2x2 supercell)** |
|---|---|---|---|---|---|---|
| $Sc_2COC$ | -160.077 | -160.098 | -160.077 | -160.077 | -160.077 | 0 |
| $Sc_2COS$ | -151.889 | -151.879 | -151.889 | -151.889 | -151.889 | 0 |
| $Sc_2CFS$ | -142.071 | -142.032 | -142.071 | -142.071 | -142.071 | 0 |
| $Sc_2CFN$ | -157.804 | -157.805 | -157.804 | -157.804 | -157.804 | 0 |
| $Sc_2COHS$ | -165.030 | -164.990 | -165.029 | -165.030 | -165.030 | 0 |
| $Sc_2COHN$ | -180.034 | -180.036 | -180.034 | -180.034 | -180.034 | 0 |
| $Sc_2CON$ | -166.402 | -166.406 | -166.398 | -166.398 | -166.397 | 2.24 |

As shown in Table S1, $Sc_2OC$, $Sc_2FN$, $Sc_2OHN$ and $Sc_2CON$ are non-magnetic (NM) structures (mark with grey shadow). $Sc_2OS$, $Sc_2FS$, and $Sc_2OHS$ also present zero magnetic moments with energy differences between their NM and FM states very small, so it can be conculude that these systems have an NM ground state.

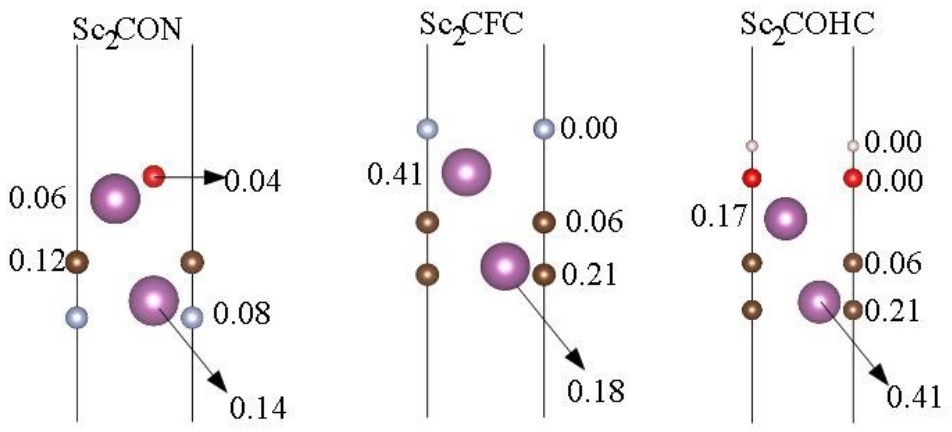

Fig S2. Individual atomic magnetic moments (μB) of $Sc_2CON$, $Sc_2CFC$, and $Sc_2COHC$.

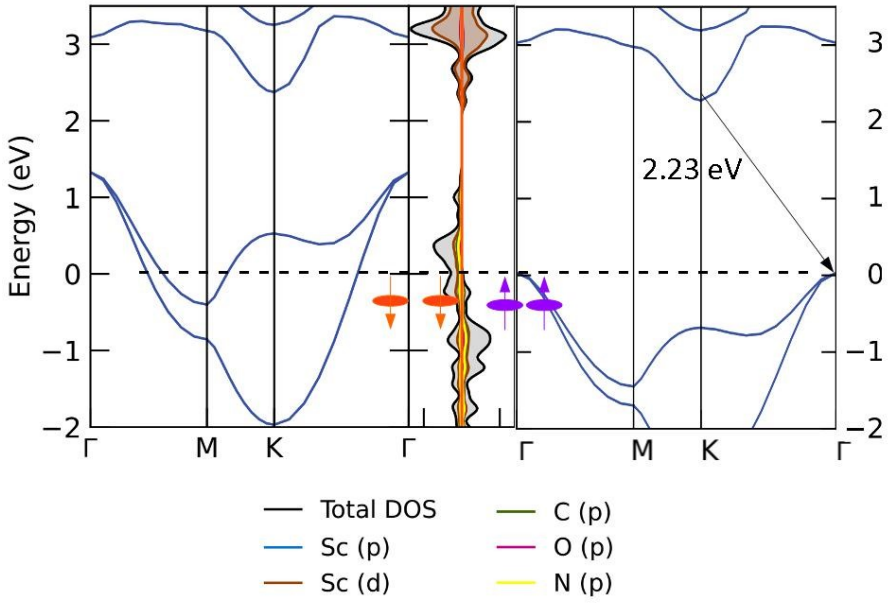


Fig S3. The band and spin-resolved density of states structures of $Sc_2CON$. The Fermi level is set at 0 eV. Bands and DOS for spin-down (up) are shown on the left (right) panels. The black arrow show the HSE06 band gap.