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

Supplementary Information:
Triarylmethyl-based 2D covalent networks: virtual screening of chemical functionalisation for optimising strain-induced property control

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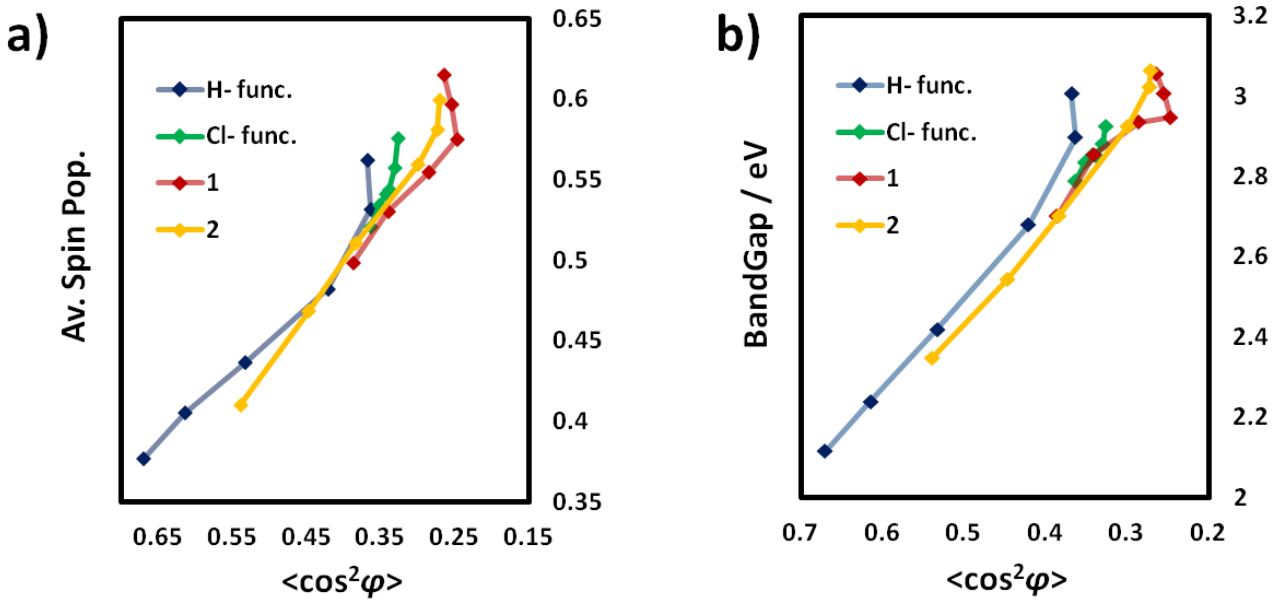

Figure S1. Average αC-partitioned spin population (**a**) and band gap (**b**) against $\langle\cos^2\varphi_i\rangle$ (where $\langle\cos^2\varphi_i\rangle = (\sum\cos^2\varphi_i)/9$ and φ_i are the twist angles of each aryl ring with respect to the corresponding αC plane) from the monotonically stretched conformations for four differently functionalized TAM 2D-networks where the three aryl rings within one of the TAM units in the unit cell have been set to the opposite helicity as compared to the rest of TAM units. Network labels correspond to those explained in the main text of the paper.

Chemical structures of considered TAMs

Below in figure S2-S8 we show the chemical structures of TAMs in the Cl_xH_y- set. TAM number 0 in the set is the fully chlorinated TAM, the so-called PTM. TAMs 0, 1-8 and 11-12 have all been experimentally synthesized (see *J. Phys. Chem.*, 1987, 91 (22), pp 5608–5616). Chemical structures of considered TAMs within the Cl_xF_y- set may be obtained upon substituting H atoms by F atoms in the TAMs shown below. Chemical structures of TAMs in the F_xH_y- set may be obtained by substituting Cl atoms by F atoms in TAMs 9, 10 and 13-19 below.

The chemical structures of all the shown TAMs have the same orientation as the red circled TAM unit in the PTM 2D-COF structure shown in Fig. 2a in the main text (i.e. the most planar aryl ring in the structures below points in a direction parallel to the direction of applied strain). Asterisks (*) indicate links with other identical TAMs within the 2D networks.

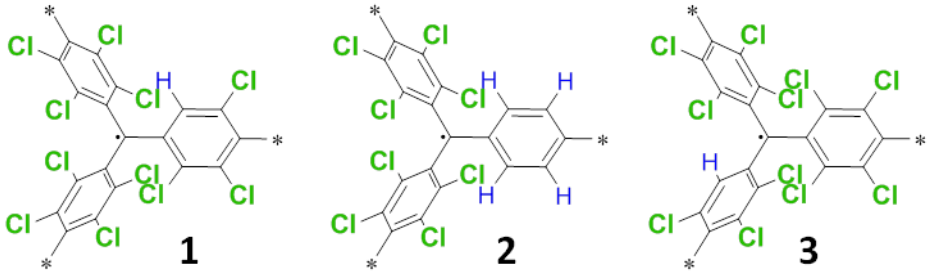

Figure S2. TAMs **1**, **2** and **3**.

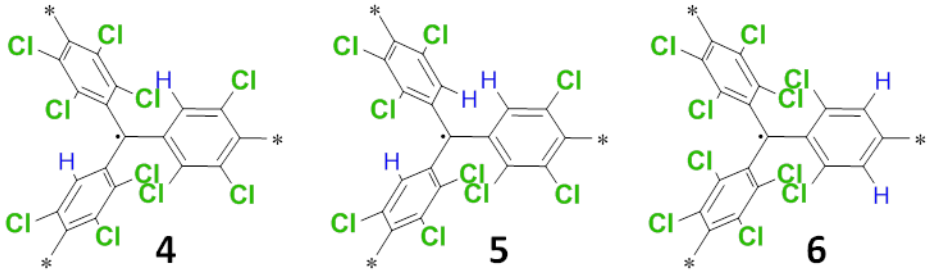

Figure S3. TAMs **4**, **5** and **6**.

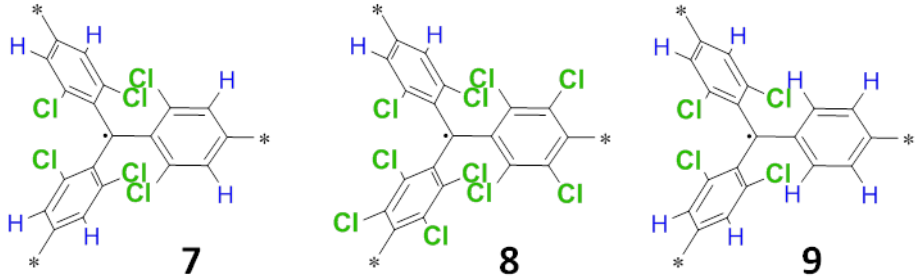

Figure S4. TAMs **7**, **8** and **9**.

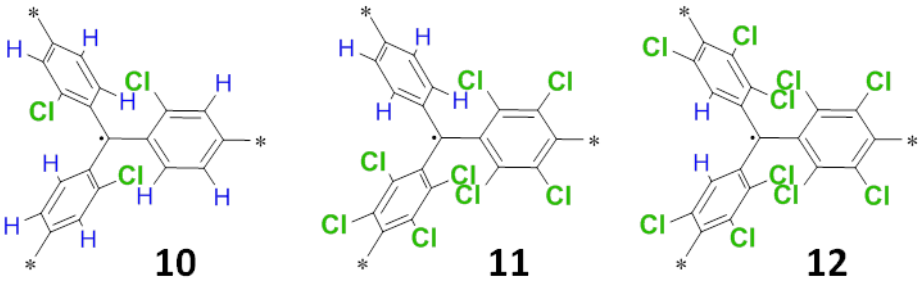

Figure S5. TAMs **10**, **11** and **12**.

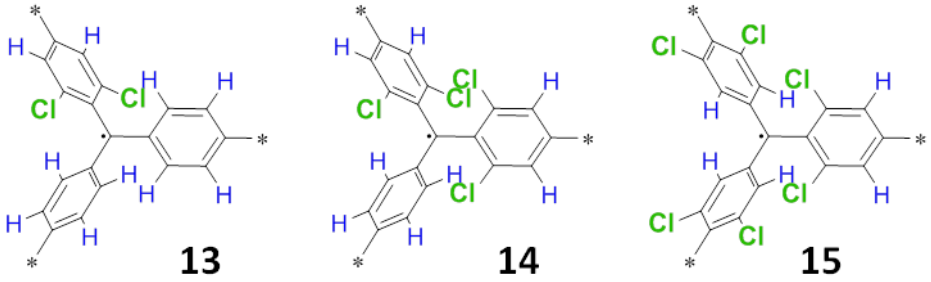

Figure S6. TAMs **13**, **14** and **15**.

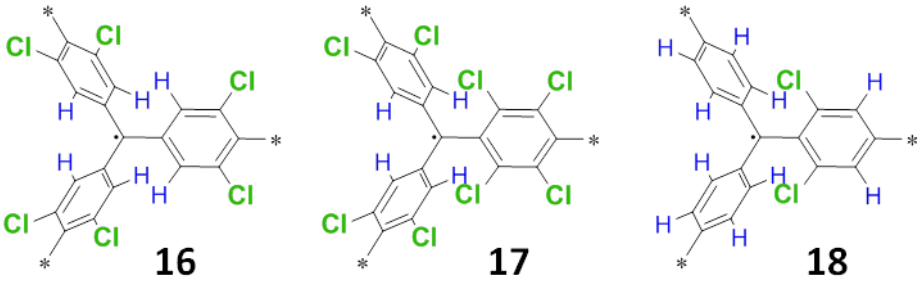

Figure S7. TAMs **16**, **17** and **18**.

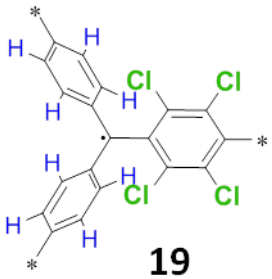

Figure S8. TAM **19**.

Structural Atomic Coordinates of PBE0 optimized TAM networks

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