Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information for An Experimental and Computational Study into the Crystallisation Propensity of 2nd Generation Sulflower

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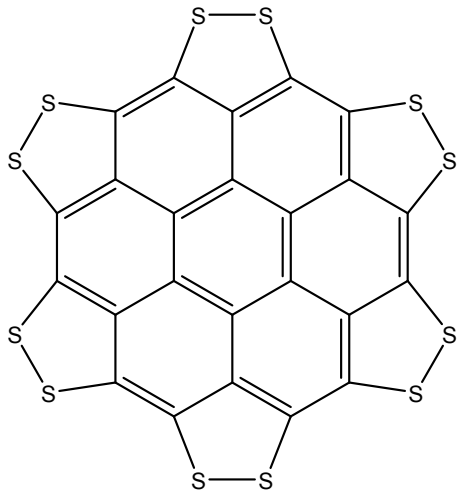
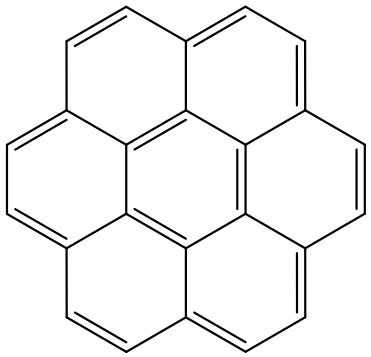
Structural Formula of Persulfurated Coronene and Coronene



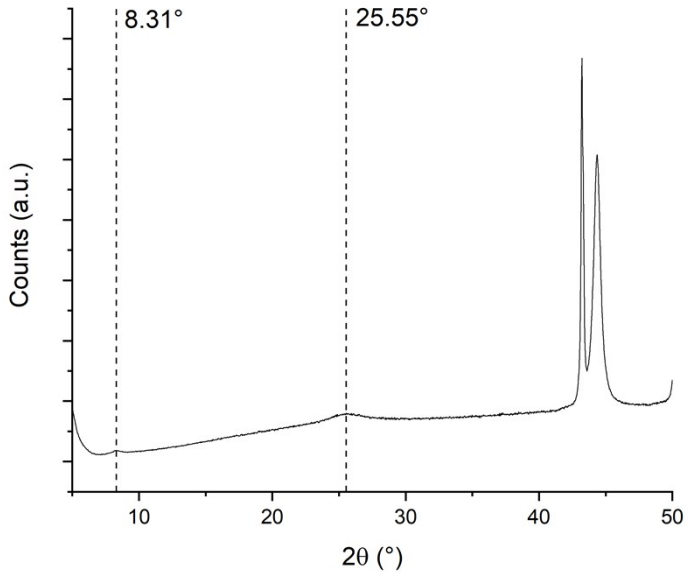
Chemical formula: $C_{24}S_{12}$ Molecular weight: 672.98



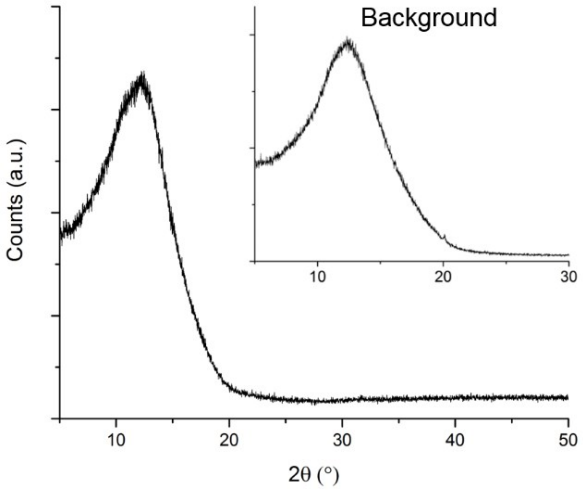
Chemical formula: $C_{24}H_{12}$ Molecular weight: 672.98

SI Fig. 1. Structural formulae, chemical formulae and molecular weights of persulfurated coronene and coronene.

Powder XRD of persulfurated coronene



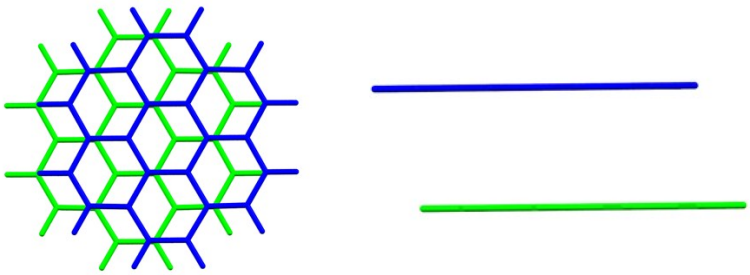
SI Fig. 2. Powder XRD data from raw persulfurated coronene powder were collected on a Bruker D8 powder diffractometer using a 20mm diameter chromium/ copper sample holder over 2θ 5-50° using Cu Kα radiation at 300 K. Peaks at <7°, 43.20°, 44.30° and >49° due to sample holder.



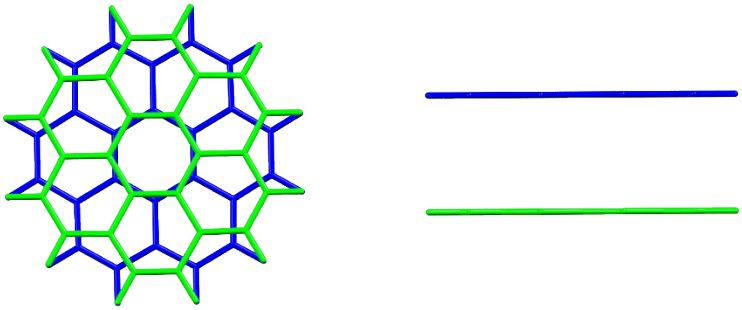
SI Fig. 3. Powder XRD data from dropcast persulfurated coronene aggregates were collected on a Bruker D8 powder diffractometer using a silicon sample holder over 2θ 5-50° using Cu Kα radiation at 300 K. Inset: Powder pattern of XRD sample holder with no sample.

Two-molecule optimizations of persulfurated coronene (PSC), coronene and sulflower

2 Molecules
Coronene – Top and Side View

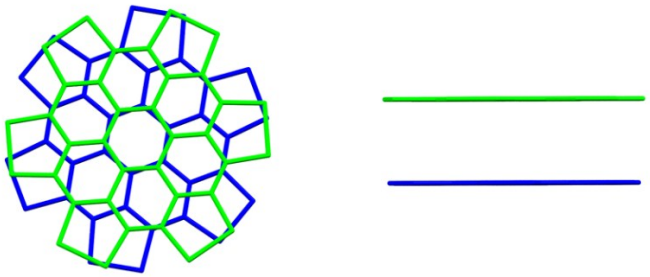


Energy ~ **-92.8 kJ.mol^{-1}** (ES = 8.8 kJ.mol^{-1}; R = 60.7 kJ.mol^{-1}; D = -162.2 kJ.mol^{-1})
Distance = **3.499 nm**; Offset = **1.376 nm**; Torsion = **0°**

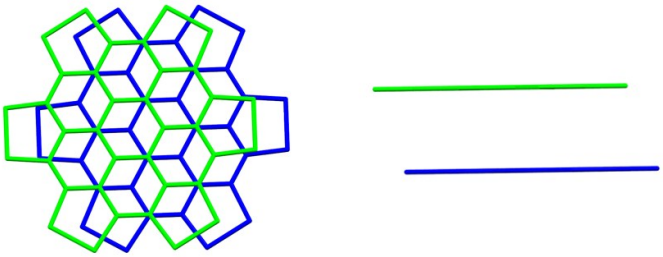


Energy ~ **-92.2 kJ.mol^{-1}** (ES = 12.8 kJ.mol^{-1}; R = 69.2 kJ.mol^{-1}; D = -164.2 kJ.mol^{-1})
Distance = **3.538 nm**; Offset = **0.0 nm**; Torsion = **30.0°**

PSC – Top and Side View

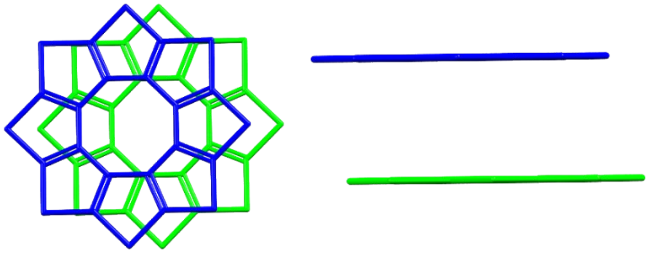


Energy ~ **-172.0 kJ.mol^{-1}** (ES = -5.7 kJ.mol^{-1}; R = 108.83 kJ.mol^{-1}; D = -275.2 kJ.mol^{-1})
Distance = **3.538 nm**; Offset = **0.0 nm**; Torsion = **16.25°**

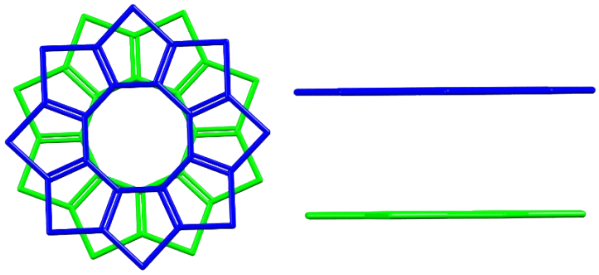


Energy ~ **-164.281 kJ.mol^{-1}** (ES = -2.1 kJ.mol^{-1}; R = 105.2 kJ.mol^{-1}; D = -267.4 kJ.mol^{-1})
Distance = **3.535 nm**; Offset = **1.293 nm**; Torsion = **0.0°**

Sulflower – Top and Side View



Energy ~ **-94.270 kJ.mol^{-1}** (ES = 2.5 kJ.mol^{-1}; R = 61.5 kJ.mol^{-1}; D = -158.3 kJ.mol^{-1})
Distance = **3.538 nm**; Offset = **1.231 nm**; Torsion = **0°**

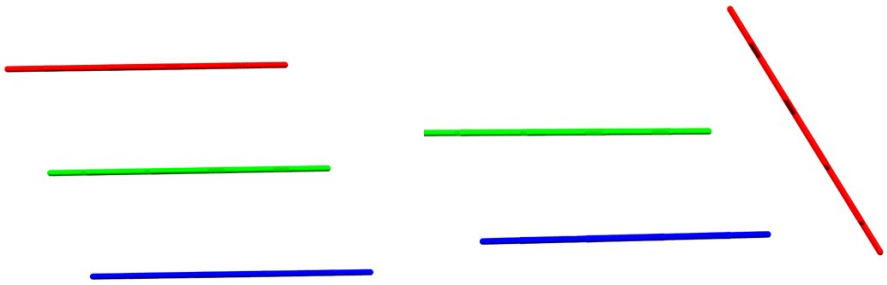


Energy ~ **-98.634 kJ.mol^{-1}** (ES = 2.2 kJ.mol^{-1}; R = 65.8 kJ.mol^{-1}; D = -166.6 kJ.mol^{-1})
Distance = **3.569 nm**; Offset = **0.0 nm**; Torsion = **22.5°**

SI Fig. 4. Final configurations after 100 optimizations of two molecules of PSC, coronene and sulflower initially positioned in different randomized starting positions performed in the ORIENT software package. Interaction potentials given plus their electrostatic, repulsion and dispersion contributions.

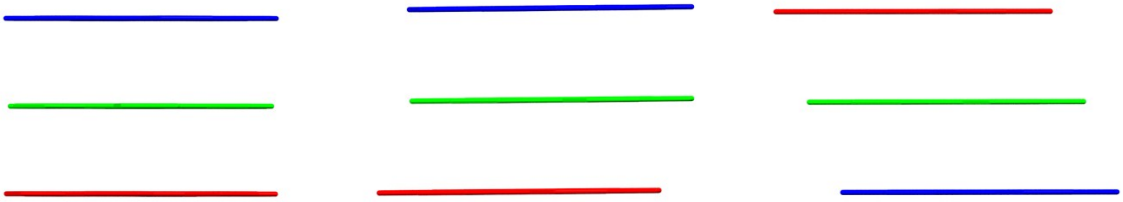
Three-molecule optimizations of persulfurated coronene, coronene and sulflower

Coronene

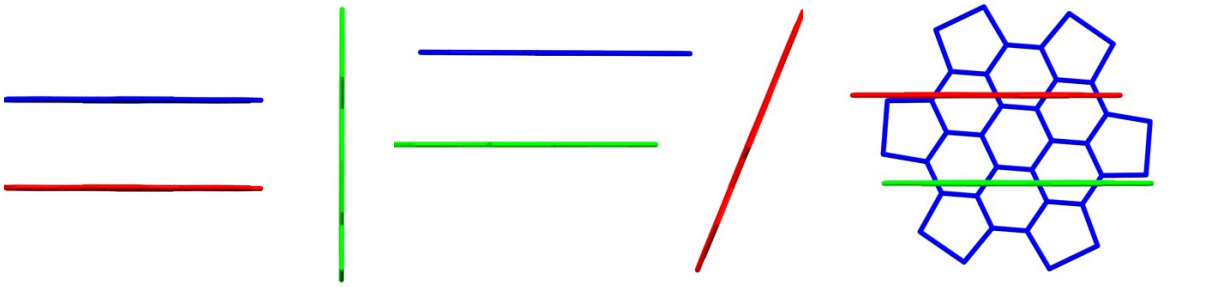


Energy = ~ -189.8 kJ.mol^{-1} Energy = ~ -141.8 kJ.mol^{-1}

PSC



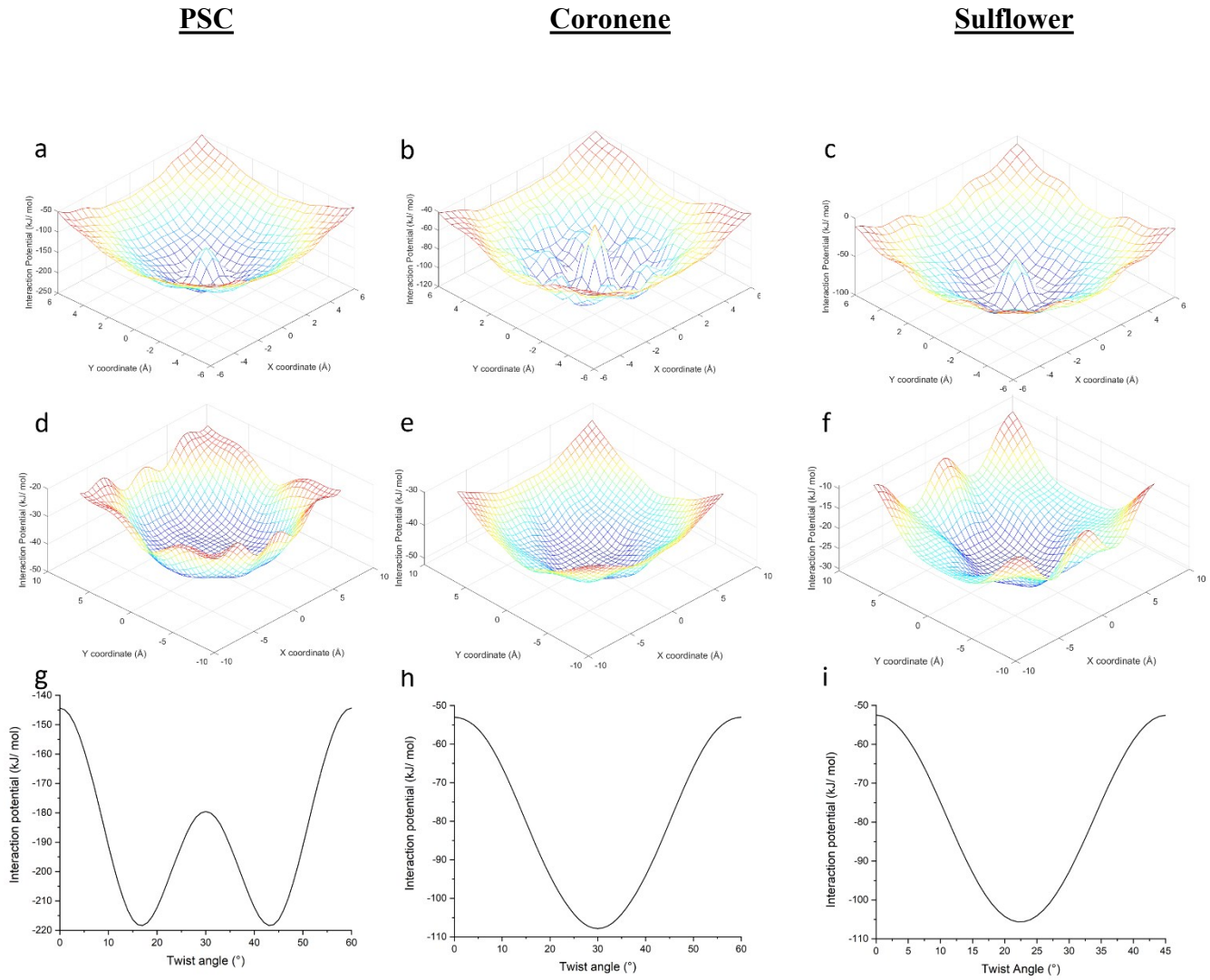
Energy = ~ -355.1 kJ.mol^{-1} Energy = ~ -347.2 kJ.mol^{-1} Energy = ~ -339.1 kJ.mol^{-1}



Energy = ~ -230.5 kJ.mol^{-1} Energy = ~ -229.0 kJ.mol^{-1} Energy = ~ -225.4 kJ.mol^{-1}

SI Fig. 5. Final configurations after 100 DFT optimizations of three molecules of PSC and coronene initially positioned in different randomized starting positions performed in the ORIENT software package, and their interaction potentials.

Interaction Potential Landscape Calculations



SI Fig. 6. Dimer interaction potential landscapes of PSC (left column), coronene (middle column) and sulflower (right column). a, b, c: Two molecules arranged in an aligned face-face configuration with one moved over a grid in the x-y plane at constant optimized z-value separation. d, e, f: Two molecules perpendicular to each other with one moved over a grid in the x-y plane at constant optimized z-value separation. g, h, i: Two molecules arranged in an aligned face-face configuration with one twisted about the center in the x-y plane at constant optimal z-value separation. Calculations performed with a b97d functional and 6-31g basis set in the Gaussian software package.