Supramolecular Polymers

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After a brief explanation of the concept of supramolecular polymers the most important construction principles based on intermolecular forces will be discussed, namely metal complexes, hydrogen bridging networks and π-π stacking. Polycondensed aromatic hydrocarbons (PAH) are prime candidates for this last type. Within the class of PAH compounds substituted hexa-peri-benzocorones (HBC, 1) occupy a prominent role. The particularly interesting perfluoroalkyl substituted derivatives present an unexpected synthetic challenge. Depending on the precise structure of these side chains (i.e. the length of the alkyl and perfluoroalkyl part, and possible ramification) and the conditions (solvent, concentration) the resulting material consists of micrometer long single stranded columnar stacks of molecules. The structural proof is based on elaborate fluorescence measurements and the cryo-SEM technique. Temperature dependent powder x-ray data provide insight in the involved stacking geometries in these columns, since closed shell PAH must adopt a staggered π-π stacking, according to theoretical calculations. In addition these calculations turn out crucial for the design of new core structures with reduced symmetry as compared to HBC, as for instance tribenzoperylene (TBP, 2), or bisanthracenocoronene (BAC, 3).

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\begin{align*}
\text{1} & \quad \text{2} & \quad \text{3} \\
R_1, R_2 = \text{H, alkyl, perfluoroalkyl}
\end{align*}
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Possible applications of the materials produced by the above structures will be discussed.