

## MS35-P27 | ENGINEERING OF SUPRAMOLECULAR COORDINATION SPHERES FOR SELECTIVE FULLERENE BINDING AND FUNCTIONALISATION

Holstein, Julian (TU Dortmund University, Dortmund, GER); Chen, Bin (TU Dortmund University, Dortmund, GER); Horiuchi, Shinnosuke (TU Dortmund University, Dortmund, GER); Hiller, Wolf (TU Dortmund University, Dortmund, GER); Clever, Guido (TU Dortmund University, Dortmund, GER)

We present a modular self-assembly system based on a new low-molecular-weight binding motif, appended by two palladium(II)-coordinating units of different steric demands, to either form a  $[\text{Pd}_2\text{L}^1_4]^{4+}$  cage or an unprecedented  $[\text{Pd}_2\text{L}^2_3(\text{MeCN})_2]^{4+}$  bowl (with  $\text{L}^1 = \text{pyridyl}$ ,  $\text{L}^2 = \text{quinoliny}$  donors). The former was used as a selective induced-fit receptor for  $\text{C}_{60}$ . The latter, owing to its more open structure, also allows binding of  $\text{C}_{70}$  and fullerene derivatives. By exposing only a fraction of the bound guests' surface, the bowl acts as fullerene protecting group to control functionalization, as demonstrated by exclusive monoaddition of anthracene. Supramolecular crystals of these systems are extremely volatile to solvent loss. Crystal quality was preserved by immediate flash cooling in liquid nitrogen and subsequent cryogenic sample handling and storage. For this study, six structures were successfully characterized by single-crystal X-ray diffraction using macromolecular synchrotron beamline P11, DESY. Challenges in structural modelling related to highly flexibility and disorder in the structures were addressed by carefully adapted macromolecular refinement protocols.