

Research Project

Design-principles and properties of networks and MOFs

Third-party funded project

Project title Design-principles and properties of networks and MOFs Principal Investigator(s) Housecroft, Catherine ; Project Members Constable, Edwin Charles ; Manfroni, Giacomo ; Organisation / Research unit Departement Chemie / Anorganische Chemie (Constable) Departement Chemie / Anorganische Chemie (Housecroft) Department Project start 01.10.2018 Probable end 31.01.2022 Status Completed We are now at a basic stage of understanding the design principles needed using divergent terpyridine ligands to direct assemblies towards 1D-coordination polymers and ladders, 2D-networks or porous 3D-architectures, the latter having the potential for small molecule uptake and storage. The project is concerned with advancing our understanding of the design principles for 3D-architectures with the aim

of better understanding the algorithms that direct a particular assembly. There is a need for *systematic* investigations of the assemblies of networks and metal-organic frameworks (MOFs). We will focus on the use of tetratopic and hexatopic oligopyridine ligands in which two or three 4,2':6',4"-terpyridine or 3,2':6',3"-terpyridine domains are connected to central core units with differing degrees of conformational freedom. The fundamental objective is to be able to control the formation of porous architectures as opposed to lower dimensionality structures. Substituent effects are important in terms of directing particular assemblies, but only with a systematic approach of altering a single structural parameter at a time can we develop much needed design principles for networks and MOFs predicated upon oligopyridine tectons.

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