

Trapping perfluoroalkyl substances in the cavity of a coordination cage adsorbent

Witold M. Bloch

Flinders University, Bedford Park, Australia

Abstract

One of the most pressing challenges in water purification is the removal of per- and polyfluoroalkyl substances (PFAS) - a large class of toxic, persistent pollutants originating from aviation firefighting foams and industrial surfactants. Human exposure to PFAS represents a significant global health and economic burden, with even low concentrations in blood linked to cancer and several chronic diseases. Current adsorbent materials struggle to remove PFAS efficiently due to slow adsorption kinetics and particularly poor affinity for short-chain PFAS. A molecular-level understanding of PFAS capture is therefore needed to guide the design of next-generation adsorbents.

In this talk, I will describe our recent work using water-soluble coordination cages based on Fujita's Pd^{II} octahedron to trap PFAS, including short-chain variants.^[1] Host-guest studies in water reveal that the cage binds C4–C8 PFAS with high affinity ($\log K \approx 5$) through a cooperative mechanism where aggregates of anionic PFAS species are bound within the cavity simultaneously. By implementing rigid *cis*-capping ligands into the cage structure, we also develop hosts with smaller cavities, capable of binding highly water-soluble C3 PFAS, which typically cannot be bound effectively by other larger cages.

We translate this host-guest chemistry into a functional material by encapsulating the Pd^{II}-based cages within mesoporous silica to create a “host-in-host” adsorbent. While the silica alone shows no PFAS affinity, incorporation of just 1 wt% cage enables >98% removal of a broad range of PFAS under flow-through filtration. The adsorption capacity correlates with host–guest chemistry, and regeneration of the material is demonstrated over five cycles.

References

C. V. I. Andersson, S. G. T. Mudiyansele, M. D. Peeks, et al. *Angew. Chem. Int. Ed.* (2026): e26027, <https://doi.org/10.1002/anie.202526027>



Bio: Wit obtained his PhD from the University of Adelaide in 2014 in the area of Metal-organic Frameworks. In 2015, he was awarded a 24-month Alexander von Humboldt Postdoctoral Fellowship which he undertook in the laboratory of Guido Clever at the University of Göttingen and TU Dortmund, Germany. During his fellowship. In 2017, Wit was awarded a University of Adelaide Ramsay Fellowship, which enabled him to return to Australia and begin his independent career. In 2019, he received an ARC DECRA Fellowship where his group developed new synthetic strategies for porous materials using supramolecular cage assemblies as building blocks. In 2022, Wit joined Flinders University as a Lecturer in Chemistry, and in 2024, he was awarded an ARC Future Fellowship. His current research focuses on the design and synthesis of coordination cages, their porous composites, and their applications in sensing and environmental remediation.