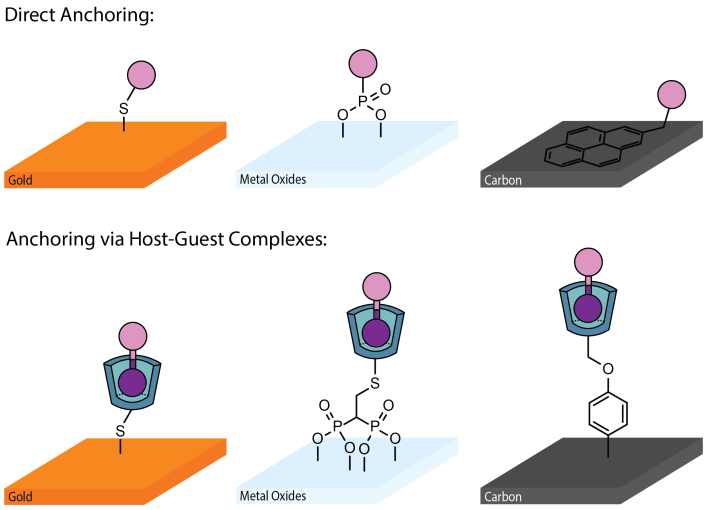
# Surface Functionalization of Carbon Substrates with Host-Guest Complexes for Electrocatalysis

I. Tunçay[1], L. Sévery[2], P. Adams[1], D. Tilley[1]*

[1]University of Zurich, Department of Chemistry, Zurich, Switzerland, [2]Université Paris-Saclay, CEA, CNRS, NIMBE, Gif-sur-Yvette 91191, France

Catalysts can be classified into two main categories: heterogeneous and homogeneous. Heterogeneous catalysts offer the advantage of greater stability, whereas homogeneous catalysts exhibit higher activity and selectivity. The advantages of both types of catalysts can be brought together by anchoring molecular (homogeneous) catalysts on electrode surfaces. The state-of-the-art immobilization strategy is to alter the structure of the molecular catalyst such that it can bind to the surface via covalent bonding, non-covalent interactions or polymerization.[1] Different alterations are necessary for different substrates and these alterations can impact the activity of the catalyst.

In our research, we explore host-guest interactions as a novel and universal immobilization strategy. Host-guest complexes form via non-covalent interactions where the guest molecule enters the cavity of the host molecule through hydrophobic interactions and/or hydrogen bonding. By using these complexes, we can immobilize the same catalyst on different substrates without having to alter the catalyst structure depending on the substrate. The only modification necessary for the catalyst is the binding unit that goes inside of the host cavity. However, the binding unit remains the same regardless of the substrate.




In our previous study[2], we successfully performed electrocatalysis on metal oxide and gold substrates by using the host-guest strategy. These studies also showed that this system leads to stable catalyst binding on the surface. Additionally we proved that the catalytic activity can be regenerated by releasing degraded catalysts from the host cavity and subsequently adsorbing fresh catalysts. Our current work focuses on extending the host-guest binding approach to carbon substrates. We are investigating if similar benefits can be achieved, whether the host-guest system has any limitations depending on different substrates and if electrocatalysis is possible.

[1] Biaobiao Zhang, Licheng Sun, *Chem. Soc. Rev.,* **2019**, 48, 2216–2264.
[2] Laurent Sévery, Jacek Szczerbinski, Mert Taskin, Isik Tuncay, et al., *Nature Chemistry*, **2021**, 13, 523-529.