UNIVERSITÀ DEGLI STUDI DI PADOVA

Title	Exploring molecular approaches to the heterogenization of metal nanoclusters for electrocatalytic applications
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Project description:

Atomically-precise metal nanoclusters represents a fundamental actor in the research about electrocatalysis of small molecules involved in sustainable fuels production. These nanosystems can indeed merge homogeneous and heterogenous catalysis: they can be synthesized with subnanometric dimensions and atomic precision, they can be functionalized at will, their solubility can be easily tuned, and, mostly, they bear a heterogeneous metal/solution interface. They can be activated both electrochemically and photochemically. They combine advantageous properties of homogeneous catalysis based on organometallic-complex and enzymatic catalysis in the sense that the surrounding of the metal core could be devised to impart selectivity to the reaction path. In the fundamental framework of electrocatalyzed processes what is still missing is a real understanding and control over the process of heterogenization of this nanocluster on the electrode surface and we believe that only a molecular approach could be instrumental to achieve this goal. Different strategies will be used to perform the clusters immobilization into different surfaces: covalent attachment, physical adsorption, integration into three-dimensional porous frameworks. Functionalized electrodes will

be electrochemically and morphologically characterized and their catalytic activity tested.
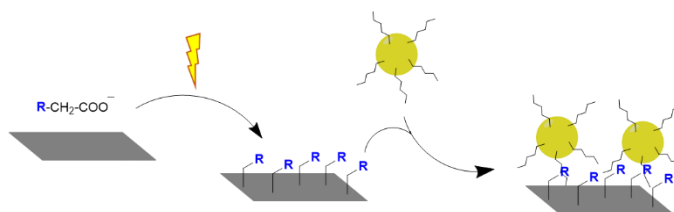
References

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Agrachev, M.; Fei, W.; Antonello, S.; Bonacchi, S.; Dainese, T.; Zoleo, A.; Ruzzi, M.; Maran, F.: *Understanding and controlling the efficiency of Au24M(SR)18 nanoclusters as singlet-oxygen Photosensitizers*. *Chem. Sci.*,

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