



PhD thesis topic

Synthesis of Heptazine-Derived Catalysts for Multielectron Reductions

In the search for **new non-innocent ligands that can act as electron reservoirs for multielectron reductions**, such as H_2 evolution (HER) or CO_2 reduction (CO_2RR), heptazine derivatives—key building blocks of graphitic carbon nitrides—offer numerous advantages. They are capable of (i) storing charges within their π -conjugated system at potentials suitable for HER or CO_2RR , (ii) stabilizing low oxidation states of metals, and (iii) offering significant versatility through the selective functionalization of their three substitutable positions, thereby allowing the electronic properties of the catalyst to be tuned.

Paradoxically, **the chemistry of heptazines remains poorly documented in the literature**, mainly due to the difficulty of controlling the reactivity of these derivatives. **The CAMPE laboratory has developed expertise in the chemistry of these compounds** and has established original methods for their functionalization. The aim of this project is therefore **to develop heptazine-based ligands and coordinate them to transition metals in order to investigate their electrocatalytic properties, particularly for HER**.

This PhD thesis will include a significant component dedicated to the **organic synthesis of new heptazine-based ligands**, as well as a second component focusing on **monometallic complexation with 3d transition metals and their physicochemical characterization**. The thesis will be conducted in close collaboration with the CEMCA (Brest), DCM (Grenoble), and BtBs (Milan) teams involved in the project. These groups will respectively investigate bimetallic complexation, electrocatalytic properties, and the rationalization of the synthesized systems through DFT studies.

The PhD will be carried out within CAMPE at the CEA Grenoble site. CAMPE is a fundamental research laboratory bringing together synthetic chemists, molecular modeling theoreticians, spectroscopists, and specialists in instrumentation. The laboratory conducts research in molecular chemistry and physical chemistry focused on the CEA's major research programs: NTE (New Technologies for Energy), nanosciences, chemistry for health and the environment. **Visits to our collaborating laboratories may be organized to share results and to receive training in, or gain exposure to, their areas of specialization.**

Candidate profile: The candidate should hold a Master's degree (or an engineering degree) in Chemistry. The candidate should have both theoretical knowledge and practical experience in organic chemistry and/or coordination chemistry, including standard purification and characterization techniques (chromatography, NMR, GC, mass spectrometry, etc.). An interest in or experience with catalysis or electrochemistry would be an advantage. A good level of English is desirable.

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