Quantum modeling of supported molecular cavities for electrocatalysis and plasmon-assisted electrocatalysis

Contract 18-month postdoctoral position starting late 2022 or early 2023

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A full-time postdoctoral research associate position is available in the Theoretical Inorganic Chemistry (*Chimie Théorique Inorganique*, CTI) team at the Institut des Sciences Chimiques de Rennes (ISCR) under the supervision of Dr. Arnaud Fihey and Dr. Mikaël Kepenekian. The position is funded through the ANR project 'Boosting efficiency and selectivity in ORR and CO_2RR by coupling metallic nanomaterials and molecular' (MARCEL) for a period of 18 months.

The activation of O_2 and CO_2 through electrochemical reduction (ORR, oxygen reduction reaction; CO_2RR carbon dioxide reduction reaction) has recently shown promising results as alternative energy conversion technologies that can produce added-value chemicals from simple and abundant feedstocks. The objectives of MARCEL are to develop a new design of ORR and CO_2RR electrocatalysts based on a molecules@materials concept. The idea is to merge the heterogeneous catalytic efficacy of Au, Ag and Cu nanomaterials with a molecular control of the interface through their deliberate surface functionalization with a molecular cavity, calixarene molecules, equipped with co-catalysts (Figure **1**). In addition, it will be taken advantage of the plasmonic properties of the targeted Au, Ag and Cu nanocatalysts to develop plasmon-mediated electrocatalysis, *i.e.* incorporate plasmonic features into the electrocatalytic systems in order to promote better performance.

The recruited postdoc will use density functional theory (DFT) based calculations as well as parametrized quantum methods (density functional tight-binding, DFTB) to characterize (i) the functionalized calixarene molecules, (ii) the grafted molecules on various nanomaterials, (iii) their catalytic properties, and (iv) explore the role of plasmons. The conduct of the project will be performed in close relationship with the teams of experimentalists in charge of the synthesis of the systems and their characterization by means of various spectroscopies.

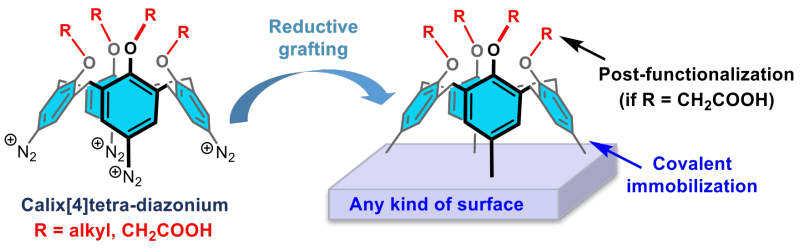
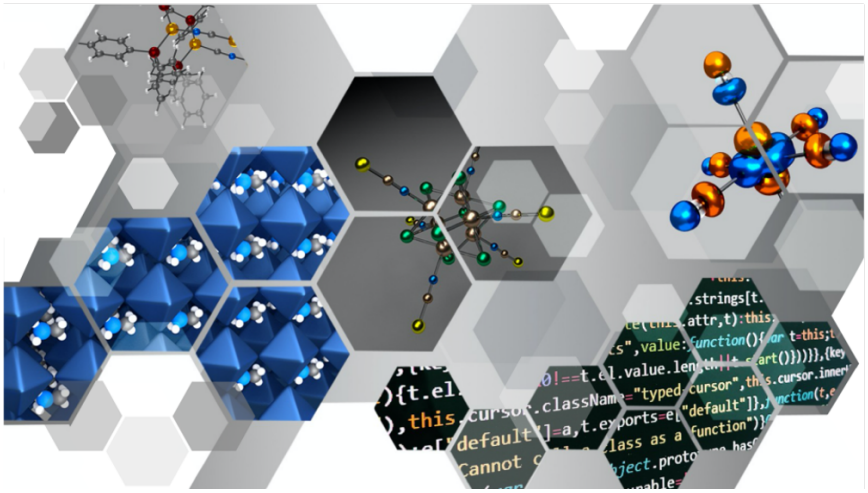


Figure 1 | Example of covalent grafting of nanosized cavity using calixarene polydiazonium salts, here calix[4]tetra-diazonium salts with simple decorating groups at the small rim.

Profile of the candidate | A PhD degree in Chemistry, Materials Sciences, Physics or related disciplines is required. We are looking for a candidate with a strong background in computational physics and/or chemistry as well as experience in DFT and/or DFTB based softwares. Previous experience in the study of supported molecules would be a plus. Complementary skills in computational material science, such as simulation code development and/or expertise using MATLAB are desirable. The candidate shall be able to demonstrate his/her expertise in the above-mentioned fields through publications in first tier journals. A good command of English, both spoken and written, is mandatory. Autonomy and communication skills are also expected.

The CTI team | The postdoctoral researcher will work in the the Theoretical Inorganic Chemistry (*Chimie Théorique Inorganique*, CTI) team at the Institut des Sciences Chimiques de Rennes (ISCR). The CTI team gathers computational chemists and physicists (15 permanent staff members, 15 students) with complementary skills, working with a broad set of quantum chemical tools, ranging from high precision ab initio wave function-based calculations to fast semi-empirical methods. CTI team members are interested in diverse type of systems, including isolated species, bulk materials and surfaces, mainly of high experimental and societal interest. The CTI team thus provides a stimulating scientific environment, also offering regular team meetings, invited seminars as well as visitors internationally recognized. Considerable local and national computing resources are available for the purposes of the scientific projects.



How to apply| Candidates should apply via the CNRS plateforme (reference UMR6226-MIKKEP-002) and join to their application an up-to-date CV and a motivation letter.