Mechanistic clarification of the interaction of nanoparticles and nanoscale coordination compounds at the interface of multiphase chemical and medicinal related processes

Aim of the Project

What do we know about the chemical interaction of nanoparticles (NPS) and nanoscale coordination compounds (NSCC) in the solid state with highly reactive nucleophiles, proteins and enzymes in solution at the solid-liquid interface? Can similar chemical processes occur on the surface of NPs and NSCC in terms of an actual ligand substitution reaction at the solid-liquid interface? As far as we know, such processes have not been investigated in detail for NSCC before. By way of *proof of principle*, we recently published a report on the ability of an Au(I) carbene complex in the solid sate to undergo a ligand substitution reaction with a stronger nucleophile dissolved in an anti-solvent.

The goal of the project is to study the chemical behavior of NPs and NSCC at the solid-liquid interface of multiphase chemical and medicinal related processes in order to gain insight into their reactivity and the underlying reaction mechanisms of such processes. The experimental work will focus on the possibility to change the structure and redox properties of NSCC through a systematic substitution of coordinated ligands by stronger nucleophiles induced by the solid-liquid interphase of multiphase reactions. The emphasis of the project will fall on the mechanistic details of the multiphase behavior of such submicron coordination compounds since very little is known about such chemical processes at present.

Description of the planned research

In this proposal, based on results recently obtained in our laboratories, we wish to tackle the problem by studying the interaction of potential ligands (in solution) with NPs and NSCC (in the solid state) during which ligand substitution reactions within the NSCC can be induced *in situ* to modify their chemical properties in the solid state. As far as we know, there are no examples in the literature where this approach has been adopted. Application of this basic principle could have far reaching advances in terms of tuning the chemical reactivity and surface properties of submicron and nanoscale coordination compounds.

The synthesis of NSCC will be carried out under ambient or anaerobic conditions depending on the air sensitivity of the compounds. A range of spectroscopic techniques will be used to characterize the synthesized NSCC in the solid state and in solution. The variety of spectroscopic techniques to be used will enable us to reveal detailed insight into the underlying chemical and physical processes that control the formation and reactivity of the NSCC.

Motivation for the research subject

As far as we know, detailed studies on the reactivity of NPs and NSCC at the solid-liquid interface of multiphase chemical processes have not been performed in an effort to systematically tune the composition and redox state of nanoscale coordination compounds. Our work will focus on the question to what extent reactants in an anti-solvent can react with NPs and NSCC in the solid state to induce ligand substitution and electron-transfer reactions. The mechanistic clarification of chemical processes that occur at the solid-liquid interface could have far reaching consequences for the systematic tuning of the properties of NPs and NSCC and their interaction with molecules of biological significance. The interaction of NSCC with potential ligands, can change bonding and oxidation state to reveal mechanistic information of the underlying process.