Project 3.8. Development of new embedding schemes for accurate quantum chemical calculations for reactions on metallic surfaces

Promotor: dr hab. Adam Kubas, prof. instytutu/ dr Aleksandra Siklitckaia

ICP PAS Group: Team 20: Cooperative Catalysis Group

WWW: http://coopcat.pl

Background:
The PhD project will focus on the development of new embedding scheme that will allow "gold-standard" coupled-cluster approach application to metallic surface chemistry. Particularly we aim to extend the scope of applications of the embedding technique developed recently for oxides (A. Kubas et al. J. Phys. Chem. Lett. 2016, 7, 4207 and A. Kubas et al. J. Chem. Theory Comput. 2018, 14, 4320) that allows not only to reach the so-called "chemical accuracy" in reaction energies (error of <1 kcal/mol) but also allows to predict spectroscopic response of the solids and adsorbed molecules (UV-VIS, IR, rRaman). Such targets are hardly reachable by existing periodic approaches based mainly on the density functional theory. Successful candidate will implement the novel embedding scheme and compare the results with existing approaches. In the next step, he/she will investigate the role of dopants in selective hydrogenation reactions using newly developed method. The PhD student will have the opportunity to visit laboratories of our international collaborators during short visits at the Karlsruhe Institute of Technology (Germany) and University College London (UK).

Aim:
(1) To develop embedding scheme that will allow to use high-level methods for metallic surface catalysis.
(2) Study the effect of dopants in nickel-catalysed chemoselective hydrogenation of unsaturated compounds.

Requirements:
-Master degree in chemistry or physics
-Experience in calculations using ab initio or force field methods
-Knowledge of at least one programming language (e.g. C++, Fortran) or scripting language (e.g. Python, Bash)
-Good command of English, both spoken and written