CSC-RUB PhD Project Proposal

Title: Quantum chemical studies of solvation effects on active sites of transition metal oxide catalysts

Sector of research: Computational Chemistry

Degree awarded: Dr. rer. Nat.

Keywords: catalysis, sustainable catalysts, solvent effects, computational chemistry, electronic structure, implicit solvent models, alcohol oxidation

Supervisor of PhD project:
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Research focus of supervisor:
The Quantum Chemistry Group at RUB has a long-standing expertise in the development and application of electronic structure methods. The group is since more than 20 years involved in the development of the TURBOMOLE program package. The three main areas of research are

- Computational studies for catalysis, which could be homogeneous or heterogeneous catalysis. For this we employ mostly density functional theory (DFT), often combined with embedding methods to account for a bulk crystal other environments.
- Implicit solvent models and general embedding methods, where the group has developed efficient approaches to combine them correlated wavefunction and response theory methods.
- Electronic spectroscopies: the group is more than 20 years engaged in the development of efficient implementations of coupled cluster response methods for electronic excitations and linear and non-linear spectra.

Publications:


Further bibliographic information on ORCID and Google Scholar.

Second Supervisor of PhD project: to be selected by the candidate
Summary of research plan:

**Background:** Today, often noble metals are used as catalysts for hydrogenation and oxidation catalysis. They are, however, costly and some of them are harmful for the environment. Possible alternatives are transition metal oxides (TMOs). Compared to noble metals, TMOs have a more complicated nuclear and electronic structure and some surface science methods that are often used to study reaction mechanisms on metals can not be applied to TMOs. This complicated the identification of reaction mechanisms and, thus, the optimization of catalysts and reaction conditions. Molecular TMO model catalysts which can be investigated with alternative methods developed for molecules provide a helpful alternative routes to investigate reaction mechanisms on TMOs catalysts.

**Study objective:** The proposed project will be concerned with the investigation of the reaction mechanism for alcohol oxidation with O$_2$ and H$_2$O$_2$ activated by molecular models for TMO catalysts like Co$_3$O$_4$ or CoFe$_2$O$_4$ in aqueous or alcoholic solution. The aim will be the identification of reaction intermediates, as for example reactive oxygen species (ROS), the understanding of their electronic structure and their characterization through vibrational spectra for comparison with experimental data. Of particular interest will be understand of the role of the transition metal atoms in the catalytic process and how the solvent affects the reaction mechanisms.

**Expected Results:** A (better) understanding of the important factors that control the reaction mechanisms, reaction rates, and selectivity for the oxidation of alcohols on TMO catalysts. This is expected to result a several papers published in peer-reviewed journals.

**Methods:** The project will use density functional theory combined with an implicit solvent model to account for the influence of the bulk solvent. Most of the calculation will be done with the TURBOMOLE program package. The calculations will be carried out of high performance computer clusters at RUB.

**Candidate Requirements:** Good English language skills. Good knowledge of electronic and molecular structure theory. Experience with the application of computational chemistry program packages. Good team player.

**For the iGSS:**
- You hold an A-grade ("very good") qualifying degree at either the level of Master or Diploma to enter the iGSS’s Track I or an A-Grade (3 yr. or, preferably, 4 yr.) Bachelor to enter the iGSS’s Track II; degrees in chemistry, physics, biochemistry, engineering, or a related discipline will be accepted.
- You are fascinated by the interdisciplinary research field Solvation Science.
- You have very good English language skills (equal to B2, oral and writing).

**Motivation for CSC application:** The Quantum Chemistry Group will provide the PhD candidate an internationally oriented research environment with cooperations with experimental and theory groups ranging from applications to method development in a worldwide used program package. He will be integrated into the structured PhD program of the Graduate School for Chemistry and Biochemistry at RUB.

**For the iGSS:**
- You will be embedded in a high-profile research environment.
- You are integrated in the International Faculty Solvation Science and will gain international work experience during a 2 – 3 months internship abroad.
- You will benefit from personal development possibilities, the entrepreneurial attitude within RESOLV and a broad spectrum of lectures as well as transferable skills courses.
- You will develop your science communication skills by presenting your research to the public.
- You are provided with funding for visiting international conferences.