

PhD position (67% TV-L E13): Modeling of photocatalytic processes for systems with strong metal support interaction

About us

In the Theoretical Chemistry group at TUM, we develop and apply electronic-structure methods to investigate reactivity with a particular focus on catalytic processes. We strive to understand catalysis in its complexity including side reactions, *operando* changes and the overall dynamics of the catalyst and its environment. Please check out <https://www.ch.nat.tum.de/theochem/> for more details.

Required qualifications

Prospective candidates

- completed their undergraduate studies (M.Sc. or equivalent) in chemistry, physics, or a related field
- are highly motivated to learn, advance and apply new theoretical methods
- are team players who are eager to communicate and learn from other group members as well as our experimental collaborators
- have at least rudimentary programming skills and prior experience with quantum-chemical software packages (e.g. VASP)
- have excellent communication skills in English

Tasks

Photocatalysis provides an economic pathway towards sustainable fuels. In this project, we aim to understand the mechanism of the photocatalytic hydrogen evolution reaction from alcohols on a TiO₂ surface decorated with small platinum clusters. While many reactions on pure titania have been analyzed and modeled in detail, the role of such cluster co-catalysts is not fully understood from a mechanistic point of view. In an initial step, we will model this reaction under UHV conditions for comparison with experimental results obtained in the group of Prof. Heiz at TUM. We will then study the effect of solvation on this reaction and optimize reaction conditions in a joint experimental/theoretical effort supported by an in-depth understanding of the reaction mechanism.

We offer

The position is fully funded, available immediately and limited to three years. TUM strives to raise the proportion of women in its workforce and explicitly encourages applications from qualified women. Applications from disabled persons with essentially the same qualifications will be given preference.

Application

Please send your CV, letter of motivation, two recommendation letters and degree certificates or transcripts of record to Prof. Dr. Christopher J. Stein (recruitment.stein@tum.de). Only complete applications will be considered. The application deadline is March 31st, 2023.

Technische Universität München

Associate Professorship for Theoretical Chemistry
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