**PhD position (67% TV-L E13): Theoretical modeling of electrocatalytic processes**

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 with excellent grades
* 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, Q-Chem)
* have excellent communication skills in English

Tasks
The theoretical modeling of electrocatalysis is a challenging task since not only the electronic structure of the catalyst but also the
environment plays a crucial role. Our group is actively developing (grand-canonical) embedding methods for metal-nanoclusters, solvation
models as well as fast electronic-structure methods for structural exploration. Open questions remain for all these topics and the precise
project will be defined with the selected PhD candidate. The project will involve method development and applications at a ratio that is
based on the candidate's prior experience and preference.

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, meaningful letter of motivation detailing your interest in the field of simulation and modeling of catalytic processes,
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 initial application deadline is June 23rd, 2023 but the position will be reopened until a
suitable candidate has been identified.

Technische Universität München
Associate Professorship for Theoretical Chemistry
Prof. Dr. Christopher J. Stein

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