PhD position at TU Wien/AT: Advanced mechanistic simulations via ab initio and machine-learning-potential molecular dynamics

A **4-year PhD position** at the Institute of Materials Science and Technology, **TU Wien**, **Austria**, is open for a **highly motivated scientist**, enthusiastic about computational materials physics and chemistry. The research project concerns current topics of *ab initio* and machine-learning potential molecular dynamics simulations of hard ceramic materials under extreme conditions, including severe mechanical loads. The position includes help with teaching and **requires and good knowledge of German.**

PhD advisor / main : Prof. Paul H. Mayrhofer, TU Wien, Austria
PhD advisor / day-to-day supervision: Dr. Nikola Koutná, TU Wien, Austria

Wider research context and aims: Wider research context and aims: The discovery of new structural materials with outstanding property combinations as well as advancing the performance of materials in use—to ultimately optimise their sustainability and biocompatibility—is the main quest of modern technologies. In this challenging task, ab initio based methods conquered an irreplaceable position, recently boosted also by machine learning. Tasks of the PhD will include development of training workflows for machine-learning interatomic potentials (for illustration see https://doi.org/10.1038/s41524-024-01252-3) as well as methodologies for mechanical simulations under experimentally-relevant conditions. The research will be carried out in a close collaboration with Dr. Nikola Koutná and her already experienced PhD student. It will be interfaced with project of a fully experimental PhD student who should start at the same time and will focus on the development of cutting-edge multicomponent materials, their thermal stability, and micromechanical testing.

Applicant's profile:

- MSc (or soon-expected MSc) in physics, chemistry, materials science, or a related field.
- Excellent command of written and spoken English & German (!).
- Proficiency in Linux environment, shell scripting, and relevant programming languages
- Experience in *ab initio* and/or molecular dynamics and/or ML techniques as a great benefit.

Application documents to be sent as a single pdf to nikola.koutna@tuwien.ac.at:

- CV
- Cover letter
- A short summary of MSc thesis
- 1–2 recommendation letters

The position is tenable from **1.6.2024**. The salary is according to the Austrian Science Fund (FWF) standard contracts for PhD candidates (annual personnel costs of approx. EUR 37.576,00 gross), which allows for a convenient life in Vienna.

For further information, please contact Nikola Koutná at nikola.koutna@tuwien.ac.at.