PhD position at TU Wien, Austria: Development and applications of machine learning interatomic potentials

A **3-year PhD position** at the Institute of Materials Science and Technology, **TU Wien**, **Austria**, is open for a **highly motivated female scientist**, enthusiastic about computational materials physics and chemistry. The position is **co-funded by the Linköping University**, **Sweden**, and will include **research visits** at this institution, as well as mentoring by and **close collaboration with Dr. Davide Sangiovanni** from the Department of Physics, Chemistry and Biology.

Project Title: Machine learning approach for high-temperature materials under extreme loads
PhD advisor: Dr. Nikola Koutná, TU Wien, Austria
PhD co-advisor: Asst. Prof. Dr. Davide Sangiovanni, Linköping University, Sweden

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. While understanding fundamental atomic-scale processes in materials (e.g. diffusion, or response to mechanical deformation) calls for quantum-mechanical accuracy, computationally affordable yet realistic enough models present a true bottleneck. Combining quantum-mechanical accuracy and computational efficiency of classical empirical potentials, machine learning interatomic potentials (MLIP) hold a great promise, however, are far from being routinely applied to real materials science problems. Within the PhD project, we will develop MLIPs for boron-based materials (transition metal diborides, MAB phases), attractive for applications as hard protective coatings for cutting tools and components used in harsh/demanding conditions, diffusion barriers in electronic devices, plasmonic materials in photothermal therapies, as well as in energy storage and conversion applications. Subsequently, we will focus on one of the main limiting factors of these materials—their low fracture resistance—and build a workflow for modelling mechanical deformation (including extreme temperatures and high loads), with the ultimate goal to provide atomic-level understanding of strengthening/toughening mechanisms and derive design guidelines for their targeted modifications.

Applicant's profile:

- MSc (or soon-expected MSc) in physics, chemistry, materials science, or a related field.
- Experience in *ab initio* and/or molecular dynamics calculations as a great benefit.
- Scripting and programming skills.
- Very good command of written and spoken English.
- Readiness to work in an international team and closely collaborate with experimentalists.

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 **1.7.2022 and will remain open until a suitable candidate is found**. The salary is according to the Austrian Science Fund (FWF) standard contracts for PhD candidates (annual personnel costs of approx. EUR 41,000.00 gross), which allows for a convenient life in Vienna.

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