MONTAN UNIVERSITÄT
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Leoben, January 20, 2017

PhD position: Atomistic study of martensitic and ordering transformations

A **3-year PhD position** is open in the Computational Materials Science (CMS) group[1] at the Department of Physical Metallurgy and Materials Testing, **Montanuniversität Leoben, Austria**.

The CMS group focuses on applying atomistic modelling techniques to the current materials science problems. The interests span from structural (structure prediction, phase stability, defects, etc.) to functional properties (e.g., surface adsorption, electronic and optical properties) and cover various material classes, from bulk intermetallic alloys to nitride and oxide thin films to carbon and gold nanostructures. A particular strength of the group lies in a close collaboration with experimentalists, both at the Montanuniversität Leoben as well as from outside.

The position is available within a MOTIF-project[2] funded by the Austrian Science Fund (FWF)[3]. The project aims on applying **first principles methods to study the ordering and martensitic transformations in the intermetallic Ti-Al-Mo system**. Particular challenges include an accurate description of the chemical disorder, diffusional properties, or finite temperature elasticity. These tasks will be addressed in a close cooperation with a partner institution Materials Center Leoben[4] and experimentalists from the Phase Transformations group[5] at Montanuniversität Leoben.

The **interested candidate** should have a Master degree (or equivalent) from Materials Science, Physics, Chemistry or a related subject, be strongly self-motivated, have good communication skills (English, German is optional), and be willing to work in a team. A prior experience with atomistic modelling is desirable, hands-on knowledge of any DFT code is not essential, but will be strongly beneficial.

Please send a CV and two recommendation letters to Dr. David Holec (`david.holec@unileoben.ac.at`). The position is available **from May 1, 2017**, and the selection of a suitable candidate will continue until filled.

[1] `http://materials.unileoben.ac.at/en/1457/`
[2] Atomistic Principles of Martensitic and Ordering Transformations in Intermetallic Alloys at Finite Temperatures
[3] `http://www.fwf.ac.at/en/`
[4] `http://www.mcl.at/`
[5] `http://materials.unileoben.ac.at/en/1374/`

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