Leoben, February 4, 2019

PhD position: Diffusion control reducing friction of nanocomposite materials

A **3-year PhD position** available **from May 1, 2019** 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 in a framework of an international basic research project funded jointly by the Austrian Science Fund (FWF)[2] and the Czech Science Foundation (GACR). The project aims on **combining first principles methods with atomistic molecular approaches** to optimise nanostructured Si-containing thin nitride coatings exhibiting reduced frictional properties. Our theoretical predictions will be corroborated by experimentally synthesising and characterising thin films. Particular challenges on the modelling side include realistic description of the interface structures and diffusion processes across such interfaces. These tasks will be addressed in a close cooperation with a project partner Advanced Materials Group[3] from the Czech Technical University in Prague, Czech Republic.

The **interested candidate** should have a Master degree (or equivalent) from Materials Science, Physics, Chemistry or a related subject, be strongly self-motivated, be fluent in English (German is optional) both in oral and written, and be willing to work in a team. A prior experience with atomistic modelling is essential, hands-on knowledge of any DFT code is strongly beneficial. Experience with Linux-based environment as well as programming/scripting skills will be considered as advantage.

The gross salary according to the FWF is € 37,680.00 p.a.

Please send a motivation letter, a CV and two recommendation letters (bundled as a single PDF document) to Dr. David Holec (david.holec@unileoben.ac.at) **before February 28, 2019**.

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[1] http://cms.unileoben.ac.at/
[2] http://www.fwf.ac.at/en/
[3] https://dce.fel.cvut.cz/advanced-materials-group

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