Leoben, March 4, 2021

PhD position: Nanostructured Carbon for Hydrogen Storage

A **3-year PhD position** available **from May 1, 2021** is open in the Computational Materials Science (CMS) group[1] at the Department of Materials Science, **Montanuniversität Leoben, Austria**.

The CMS group focuses on applying quantum-mechanical and atomistic modelling techniques to tackle current materials science problems and challenges. 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 close collaboration with experimentalists, both at the Montanuniversität Leoben as well as numerous national and international institutions.

The position is one of several University-funded positions aimed at establishing a world-leading group of experts in the field of hydrogen storage which will bridge basic research to industrial applications. This specific PhD project aims at the quantum-mechanical and atomistic description of interactions between carbon nanostructures functionalized with metallic catalysts and/or organic functional groups to enhance a capacity for hydrogen adsorption and storage. Special focus will be paid to the impact of local structural/binding motifs and defects, with the ultimate goal to upscale the modelling methods for large-scale nanoporous simulations.

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, be a good team player and possess the ability for independent work and scientific publication. A prior experience with atomistic modelling is essential, hands-on knowledge of any DFT code as well as molecular dynamics (MD) and/or Monte Carlo (MC) is strongly beneficial. Excellent programming skills in particular using Python, experience with Linux/Unix systems as well as compiling codes at high-performance computer clusters will be considered as an advantage.

The gross salary for 40 hours/week contract is € 2 971.50 (14× per year).

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 March 25, 2021**.

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[1] http://cms.unileoben.ac.at/

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