

The Dep. of Functional Materials headed by Prof. O. Gutfleisch at the Institute of Material Science at TU Darmstadt is offering a

Doctoral Researcher (PhD) Constructing Sm-X-Fe-M-Z Multielement Phase Diagrams Using Machine Learning

75 % with a fixed-term contract of 3 years

High-performance permanent magnets are essential for electric vehicles and wind turbines. Currently, this demand is satisfied by anisotropic NdFeB-based magnets. The EU's climate goals require a significant increase in green energy technologies, driving up the production of NdFeB-based magnets. However, the elements used in these magnets are critical and strategic. To meet this demand, we need to develop a resource-efficient alternative magnet. SmFe₁₂-based (1:12) magnets, which have the highest Fe content among the 4f-3d compounds, can potentially replace or complement NdFeB-based magnets. However, realizing the large coercivity with high magnetization is the main bottleneck for their practical application. This can be overcome by finding the phase equilibrium between the SmFe₁₂ and low melting point phases while keeping the phase stabilizer elements. This equilibrium combined with the optimum processing technique will lead to an optimum microstructure where 1:12 grains are isolated with an intergranular phase.

The position is hosted by the internationally renowned Functional Materials Group, which focuses on the development of resource-efficient functional materials. In our research, we investigate several phase stabilizer elements and construct phase diagrams using an active learning pipeline. This pipeline begins with data collection from existing literature, applies appropriate machine learning models to predict unknown regions, and evaluates predictions through accuracy testing and experimental validation. This project is a part of ERC project MAG-TOOL (https://www.mawi.tu-darmstadt.de/fm/outreach_fm/news_fm/news_fm_details_93888.en.jsp). Our research contributes to the development of novel magnets from fundamental mechanisms to applications. Additional research topics include magnetocaloric materials for hydrogen liquefaction, magnetic materials for biomedical and catalytic applications, with a focus on synthesis, additive manufacturing, characterization, and modeling of magnetic, thermal, and microstructural properties.

Your tasks within the project will involve investigating the Sm-X-Fe-M-Z phase diagrams, focusing on the 1:12 phase and its neighboring phase areas using an active learning pipeline. You will perform literature searches and experimentally synthesize samples using induction melting and additive manufacturing for bulk samples and melt spinning for ribbons to seek phase equilibrium. Additive manufacturing will be used in particular to synthesize the bulk material with composition gradient. You will present the results in international scientific journals, conferences, and regular project meetings.

Your profile: Requirements include an excellent scientific degree (master's or equivalent) in Materials Science, Physics, or Chemistry. Ideally, you have experience with the synthesis and characterization of metallic or magnetic materials, in particular in additive manufacturing. Knowledge of programming is considered an advantage. You must have very good English skills (fluent in both spoken and written) and strong communication competencies. We expect you to integrate into our interdisciplinary team, actively contributing to the overall progress of the project's objectives while pursuing your thesis with high motivation and independence. You should be highly motivated to publish your results, present them at international project meetings and conferences, and enjoy working in interdisciplinary and international teams.

We offer: The opportunity to work towards a PhD degree on a cutting-edge research topic in the field

of functional materials for energy conversion and excellent working conditions in an international team with integration into a scientific network of well-renowned experts of the magnetic materials community. The Technical University of Darmstadt offers a varied, diverse working environment, independent work, demand-oriented training opportunities and individual personnel development. Flexible working hours, company health management, and the compatibility of family and career are a matter of course. In addition, you will receive free travel authorization for local and regional transport in the area of the state of Hesse (LandesTicket Hessen) according to the applicable regulations. All university employees can use the offer of deferred compensation in favor of a "Job Rad" leasing model.

The Technische Universität Darmstadt intends to increase the number of female employees and encourages female candidates to apply. In case of equal qualifications applicants with a degree of disability of at least 50 or equal will be given preference. Wages and salaries are according to the collective agreements on salary scales, which apply to the Technische Universität Darmstadt (TV-TU Darmstadt). Part-time employment is generally possible. Applications (all in a single PDF-file) should be sent including all usual documents, stating the above identification number, in the form of a pdf by e-mail to info@fm.tu-darmstadt.de. If you have any questions, please contact Dr. Pelin Tozman (pelin.tozman@tu-darmstadt.de) or Prof. Oliver Gutfleisch (oliver.gutfleisch@tu-darmstadt.de). For the website of the FM group, see www.mawi.tu-darmstadt.de/fm.