CRC/TRR 270

# HoMMage

TECHNISCHE UNIVERSITÄT DARMSTADT

UNIVERSITÄT DUISBURG ESSEN

*Offen im Denken*

## Hysteresis Design of Magnetic Materials for Efficient Energy Conversion

**Tuesday, 9 May 2023, 9:00 s.t., TU Darmstadt, via Zoom and in person**


**Dr. Heike C. Herper**

**Division of Materials Theory**

**Department of Physics and Astronomy**

**Uppsala University, Uppsala Sweden**


# Data driven design of new permanent magnets


### Abstract:

Magnetic materials play a key role in many “green energy“ applications, such as electric transportation, wind power generation, but they are also present in many other “every day” devices such as audio equipment, actuators, medical supplies and many more. The increasing interest in environmentally friendly technologies has triggered the search for new magnetic materials being ecologically and economically superior to the currently existing rare-earth magnetic materials.

Computational design has been proven to be a powerful tool for this purpose. In the studies presented here, we combine big data searches and high throughput calculations to identify new candidates for permanent magnets. Starting from a pool of more than 1000 phases we apply a combination of filters to extract possible candidates for new permanent magnets or magnetic refrigeration. Phases which pass all filter criteria are investigated in detail using a combination of first principles electronic structure methods and thermodynamic modelling [1,2,3]. Regarding new permanent magnets a promising example has been found and successfully synthesised showing the characteristics of a good permanent magnet [4]. Funded by the Swedish Strategic Research Foundation (SSF), (Grant EM16-0039), STandUpp, eSSENCE, ERC (synergy grant FASTCORR, project 854843), Swedish National Infrastructure for Computing (SNIC) at PDC and LIU.



[1] A. Vishina, O.Y. Vekilova, T. Björkman, A. Bergman, H.C. Herper, O. Eriksson, Physical Review B **101**, 094407 (2020); [2] A. Vishina , D. Hedlund, V. Shtender,… ,H.C. Herper, Acta Materialia **212**, 116913 (2021); [3] M. Marathe and H. C. Herper, accepted for publication in Physical Review B (2023); [4] A. Vishina, O. Eriksson, H.C. Herper, Materials Research Letters **11** (1), 76-83 (2023)


### About the speaker:

Heike Herper got her education in physics and materials science from the Gerhard Mercator University in Germany (now University of Duisburg-Essen) and at the Center for Computational Materials Science at the TU Vienna (Austria) where she worked after her PhD in 2000. Further, she was visiting scientist at the Los Alamos National Laboratory (USA). In 2013 she joined the Materials Theory group at Uppsala University (Sweden) where she received a docentship in 2022. Her research area are functional materials and their understanding and prediction from the atomic modelling. Special focus is on materials for magnetic applications (permanent magnets, magnetocaloric materials, spintronics) but also includes theoretical spectroscopy.