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TECHNISCHE UNIVERSITÄT DARMSTADT

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Offen im Denken

Hysteresis Design of Magnetic Materials for Efficient Energy Conversion

Tuesday, 12 March 2024, 9:00 s.t., UDE, in Person and via Zoom

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Perspectives for machine-learning applied to data-rich experiments on complex materials

Abstract:

The on-going hype of machine-learning promises that any insight can be gained by computers when you have enough data to learn from. Experiments that resolve the structural and chemical complexity of materials meet this demand: single experiments can provide gigabytes or terabytes of data, and the data is known to encode the underlying materials physics in a way that is somehow amenable to understanding. Such data is often noisy, but contains characteristic patterns in space or time that relate to the material's performance. Reversely, machine-learning techniques are urgently needed to actually process the data in a way that extracts relevant information for our human understanding of materials. I will show examples from scanning transmission electron microscopy and atom probe tomography, and highlight how to shape and adapt existing algorithms to perform data evaluations that target useful materials science concepts.

About the speaker:

Christoph Freysoldt studied Chemistry at Leipzig university from 1997-2002, with a one-year break at Uppsala University in 2000-2001. He then moved to the Fritz Haber Institute of the Max Planck Society to pursue his PhD in Physics, which he received from the Free University Berlin in 2007. In the same year, he started at Max-Planck Institut für Eisenforschung (MPIE) in the Computational Materials Design Department to work on point defect simulations, which would become one of his major research areas. At MPIE, he was assigned scientific group leader in 2007 and head of the department IT group in 2012. In 2009, he also became responsible for the development of the department's own code for density functional theory (DFT) calculations, named SPHInX.

Christoph Freysoldt's research focuses on computing properties of point defects in semiconductors and insulators using DFT, method development in the context of ab initio electronic structure theory, the study of electrified surfaces at the atomic scale, and the use of machine learning algorithms for exploring data-rich experiments such as APT and STEM. In 2010, he received the Volker-Heine Young Investigator award for proposing a reliable correction scheme for artificial Coulomb interactions in charged-defect supercell calculations, which quickly became state of the art in the field.