

## **REPM 2016**



TECHNISCHE UNIVERSITÄT DARMSTADT

## 28 August to 1 September 2016 in Darmstadt, Germany

Abstract Alexander Edström:

## From the electronic structure theory of magnetocrystalline anisotropy to novel rare-earth free permanent magnets

We discuss the electronic structure theory of magnetocrystalline anisotropy in the context of finding novel rare-earth free permanent magnets. In particular we use density functional theory (DFT) based calculations to show how uniaxial strain and alloying can be used to tune the properties of 3d-based magnets. Additionally we provide recent examples of how to further improve such materials by adding, for example, 5d-elements.