GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Fachbereich Physik
Institut für Theoretische Physik

Condensed Matter Theory Seminar

Subject:	**Optimizing the finite-temperature magnetic anisotropy and magnetization in 4f-3d intermetallics: combined studies of ab initio modeling and solutions of the low-energy many-body problem therein**
Speaker:	Mr. Munehisa Matsumoto, National Institute for Materials Science (NIMS), Tsukuba/Japan
Date & time:	**Friday, August 26th, 2016 at 3:15 p.m.**
Venue:	**Seminar room 1.114**

Abstract:

The rare-earth permanent-magnet as exemplified by the champion Nd-Fe-B magnet are made of 4f-3d intermetallics where the strong magnetic anisotropy originating in localized 4f-electrons are transmitted to the 3d-electron magnetization via 5d-electron-mediated indirect exchange interactions. The temperature dependence of the intrinsic magnetic properties of a given permanent-magnet material in its practical operation temperature range spanning several hundreds of Kelvins can be modeled with a multiple-sublattice classical spin model: part of the sublattices carries spins with the single-ion anisotropy of 4f electrons and the others represent the dominant 3d-3d exchange interaction, which are defined on a lattice mimicking the realistic crystal structure with all of the model parameters basically derived from first principles. Numerically exact Monte Carlo studies of Nd2Fe14B [1] and NdFe12Nx [2], where the latter is a material that intrinsically goes beyond the former which is today's champion magnet compound, show how the operation-temperature magnetic anisotropy can be sensitive to the fine-tuning of 5d-mediated indirect exchange interaction, potentially leading to a low-cost solution for the high-temperature applications of rare-earth-based permanent magnets. Secondly, our LDA+DMFT studies combined with experimental fabrication and measurements for Ce-Cu-Co intermetallics are described as another approach utilizing Ce with an appropriate valence control on its 4f-electron to cost-effectively yield the desired magnetic anisotropy at finite temperatures.

References:

[1] Y. Toga, MM, S. Miyashita, H. Akai, S. Doi, T. Miyake, A. Sakuma, arXiv:1606.00333
[2] MM, H. Akai, Y. Harashima, S. Doi, T. Miyake, J. Appl. Phys. 119, 213901 (2016)