

Magnetic properties of La doped rare earth permanent magnetsM. Hoffmann¹, M. Matsumoto¹, and H. Akai²¹ *Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan*

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Powerful permanent magnets are a crucial component in electric motors and generators, while the most powerful magnets available nowadays are alloys of rare-earth (RE) elements like Nd or Dy and magnetic transition metal (TM) elements like Fe or Co. Unfortunately, the availability of the RE elements of the best magnets is strongly limited while they became rather expensive in production. Therefore, different paths are undertaken in order to find better or cheaper permanent magnets. We study computationally the effect of La doping on the magnetic properties of permanent magnet.

The major physical properties under consideration are the coercive field strength, the magnetization, and the Curie temperature. In terms of computation methods, we are looking for the magnetic moments, the magnetic coupling, the magnetic anisotropy and the Curie temperature. These quantities and their dependence on the doping have to be at first better understood and in a second step optimized for a good performance of the magnets.

We use a multi-code approach for the theoretical investigation utilizing the Korringa-Kohn-Rostoker method, the Vienna *ab initio* simulation package (VASP) and Open source package for Material eXplorer (OpenMX). We found significant changes in the calculated magnetic properties when mixing La with RE. Looking at the formation energy of the compounds identifies possible stable concentration regimes where new compounds could be synthesized.