Ab-initio study of magnets

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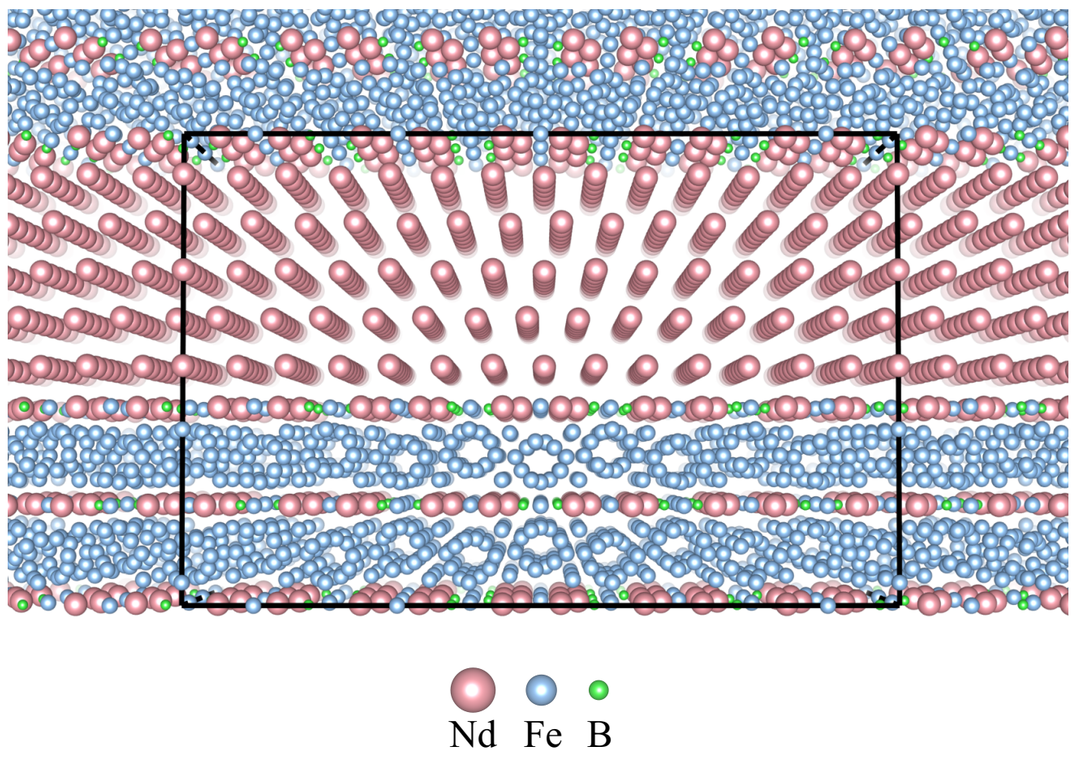
1. Introduction

Development of new hard magnets avoiding the use of dysprosium is desired to reduce the risk of the raw-material supply. A promising first step is to understand the mechanism of high performance of existing magnets, specifically Nd-Fe-B sintered magnets. Since the performance of sintered magnets cannot be understood by the knowledge of main-phase single crystals, we perform large-scale first-principles calculations of Nd-Fe-B microstructure interfaces using the K computer. In addition, a few intermetallic compounds are also studied to acquire knowledge, which should be useful for theoretical design of new compounds as candidates for alternative permanent magnets.

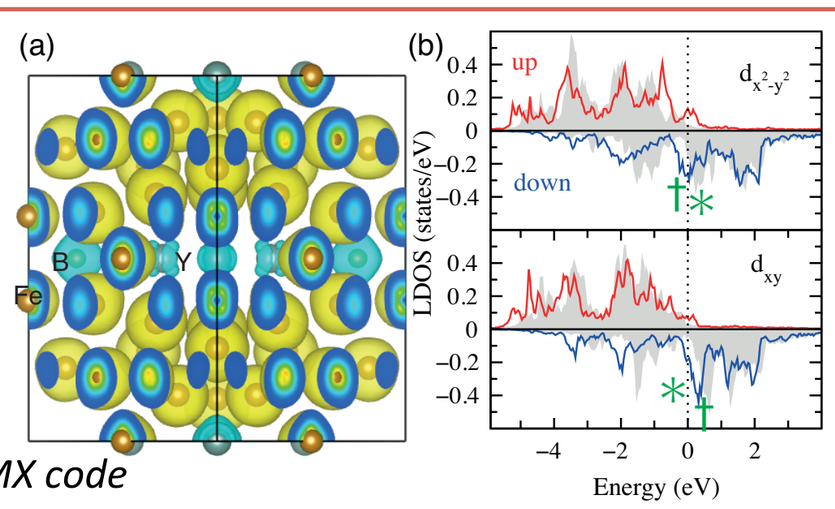
2. Nd-Fe-B microstructure interfaces

Interfaces between the main phase ($Nd_2Fe_{14}B$) and a sub phase (dhcp Nd) including 2,700 atoms with c.a. 36,000 valence electrons within the unit cell are calculated as massively parallel computations using approx. 20,000 cores of the K computer by the OpenMX code [www.openmx-square.org]. First-principles atomic-structure optimization is performed using Krylov-subspace order-N calculations. Local magnetic properties at the interface are compared with those inside the bulk main phase.



D. Hirai, T. Ozaki, S. Tsuneyuki, and Y. Gohda, in preparation.

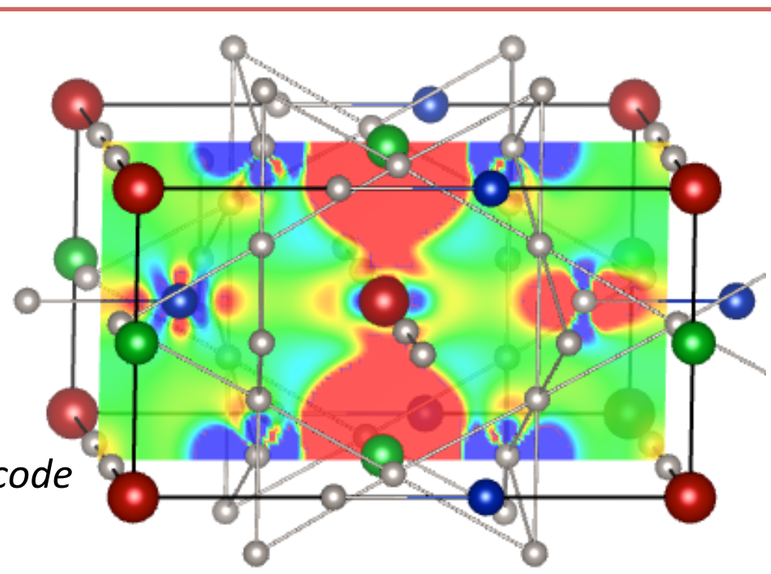
3. Toward design of new magnets



OpenMX code

Role of itinerant electrons clarified for strain effects on the magnetic anisotropy in $Y_2Fe_{14}B$.

Z. Torbatian, T. Ozaki, S. Tsuneyuki, and Y. Gohda, Appl. Phys. Lett. **104**, 242403 (2014).



QMAS code

Large magnetization and anisotropy of $NdFe_{12}N$

T. Miyake, K. Terakura, Y. Harahima, H. Kino and S. Ishibashi, JPSJ **83**, 043702 (2014)