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**Electronic Structure Calculation of Permanent Magnets using the KKR Green's Function Method** SHOTARO DOI, HISAZUMI AKAI, ISSP, The University of Tokyo — Electronic structure and magnetic properties of permanent magnetic materials, especially  $\text{Nd}_2\text{Fe}_{14}\text{B}$ , are investigated theoretically using the KKR Green's function method. Important physical quantities in magnetism, such as magnetic moment, Curie temperature, and anisotropy constant, which are obtained from electronics structure calculations in both cases of atomic-sphere-approximation and full-potential treatment, are compared with past band structure calculations and experiments. The site preference of heavy rare-earth impurities are also evaluated through the calculation of formation energy with the use of coherent potential approximations. Further, the development of electronic structure calculation code using the screened KKR for large super-cells, which is aimed at studying the electronic structure of realistic microstructures (e.g. grain boundary phase), is introduced with some test calculations.

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