First principles investigation of some rare-earth free permanent magnets

A Thesis Submitted for the Degree of

Doctor of Philosophy

in the School of Basic Sciences

by

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Declaration by the Research Scholar

I hereby declare that the entire work embodied in this Thesis is the result of investigations carried out by me in the **School of Basic Sciences**, Indian Institute of Technology Mandi, under the supervision of **Dr. Arti Kashyap** and that it has not been submitted elsewhere for any degree or diploma. In keeping with the general practice, due acknowledgements have been made wherever the work described is based on finding of other investigators.

Place: Signature:

Date: Name:

Declaration by the Research Advisor

I hereby certify that the entire work in this Thesis has been carried out by **Rohit Pathak**, under my supervision in the **School of Basic Sciences**, Indian Institute of Technology Mandi, and that no part of it has been submitted elsewhere for any Degree or Diploma.

Signature:

Name of the Guide:

Date:

ABSTRACT

Development of rare-earth free, permanent magnetic materials plays a major role in today's world of technological advancement. Permanent magnets find applications in electric motors, hard discs drive, loudspeakers and many more. Sm-Co and Nd-Fe-B are two very famous rare-earth based permanent magnets in terms of commercial applications because of their very good hard magnetic properties. But due to limited resources and volatility of price of rare-earth metals, there is a high demand for rare-earth free, permanent magnets from technological and scientific communities since the last few decades.

First principles-based density functional theory (DFT) is one of the crucial realms of research for designing tailor-made materials with specific properties. DFT calculations have proven to be very useful and powerful tool in understanding atomistic origin of magnetic properties of permanent magnets as well. These calculations not only help understand the experimental findings but also open up new directions for designing the experiments. DFT calculations have the capability to predict and explore tuning of various electronic and magnetic properties of materials.

This dissertation investigates the electronic structure and magnetic properties of few rare-earth free permanent magnets which are also experimentally realized. Out of several known types of rare-earth free permanent magnet materials, our investigation was focused on three different kinds of materials: (i) transition metal borides (iron doped $Ti_3Co_5B_2$), important in context of alnico magnets, (ii) two cobalt based intermetallic compounds (Co_2TiSi and $Co_{1+x}Sn$) and one silicide (Co_3Si) and (iii) binary (four phases of Fe-Pd) and ternary (four phases of boron doped Fe-Pd) intermetallic compounds. All of them are important and potential candidates for rare-earth free permanent magnets.

Initial two chapter of the dissertation deals with the introductory background of rare-earth free permanent magnets and with theoretical methodologies for studying and understanding various magnetic properties relevant to permanent magnetism.

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LIST OF PUBLICATIONS

THE FOLLOWING PUBLICATIONS AND MANUSCRIPTS ARE BASED ON THIS THESIS:

- **R. Pathak**, I. Ahamed, W. Y. Zhang, S. Vallopilly, D. J. Sellmyer, R. Skomski, and A. Kashyap; "Half-metallic magnetism in $Ti_3Co_{5-x}Fe_xB_2$", AIP Advances 7, 055713 (2017).
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