

# The enhancement of the magneto-optical effects by Bi in (Rh/Ir)<sub>2</sub>MnAl – first-principle study

Dominik Legut<sup>1</sup> and Eithiraj R. Dashinamoorthy<sup>1</sup>

<sup>1</sup>*Nanotechnology Centre, VSB-TU Ostrava, Ostrava, Czech Republic*

We have performed first-principle calculations to investigate structural, electronic and optical properties of (Rh/Ir)<sub>2</sub>MnAl and (Rh/Ir)<sub>2</sub>MnBi Heusler alloys using density functional theory [1]. Three spin orderings, i.e. ferromagnetic and antiferromagnetic along [001] and [111] crystal axis were considered. In contrast to the experimental study [2], where the antiferromagnetic ordering was detected with high Neel temperature, our calculations show that the Rh<sub>2</sub>MnAl possesses the lowest total energy with ferromagnetic ordering. Therefore, considering the ferromagnetic ordering we investigate the enhancement of the Kerr rotation and ellipticity by the substitution of Al by Bi within 0-10 eV energy range.

## References:

- [1] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
- [2] H. Masumoto and K. Watanabe, J. Phys. Soc. Jpn., 32, 281-281 (1972).