

# Physikalisches Kolloquium

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»Rational Design of New materials:  
from Topological Insulators to Spintronics«

*Einführung: W. Wulfhekel*

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Heusler compounds are a remarkable class of intermetallic materials with 1:1:1 (often called Half-Heusler) or 2:1:1 composition comprising more than 1500 members [1]. Today, more than a century after their discovery by Fritz Heusler, they are still a field of active research. New properties and potential fields of applications emerge constantly; the prediction of topological insulators is the most recent example [2]. Surprisingly, the properties of many Heusler compounds can easily be predicted by the valence electron count or within a rigid band approach. Their extremely flexible electronic structure offers a toolbox which allows the realization of demanded but apparently contradictory functionalities based on a virtual lab approach. The subgroup of more than 250 semiconductors is of high relevance for the development of novel materials for energy technologies. Their band gaps can readily be tuned from zero to 4 eV by changing the chemical composition. Thus, great interest has been attracted in the fields of thermoelectrics and topological insulator research. Ternary materials based on multifunctional properties, i.e. the combination of two or more functions such as superconductivity and topological edge states will revolutionize technological applications. The design scheme for topological insulators from the view point of bands and bond will be presented.

The wide range of the multifunctional properties of Heusler compounds is reflected in extraordinary magneto-optical, magneto-electronic, and magneto-caloric properties. Tetragonal Heusler compounds  $Mn_2YZ$  as potential materials for STT applications can be easily designed by positioning the Fermi energy at the van Hove singularity in one of the spin channels [3]. A high calculated magnetic anisotropy energy (MAE) is the sufficient condition for a material with perpendicular magnetocrystalline anisotropy (PMA). Materials with saturation magnetizations of 0.2 – 4.0  $\mu_B$ , high Curie temperatures of 380 – 800 K, high spin polarizations, PMA, and required lattice constant matching with MgO can be realized with ferri- or ferromagnetic Heusler-related compounds. Such materials are strongly recommended for the spin transfer torque magnetic random access memory (STT-MRAM) data storage and the spin torque oscillators (STO) for telecommunication. Additionally the first spin gapless semiconductor is realized in  $Mn_2CoZ$ .

[1] Simple Rules for the Understanding of Heusler Compounds, Tanja Graf, Stuart S. P. Parkin, and Claudia Felser, Progress in Solid State Chemistry (2011), doi:10.1016/j.progsolidstchem.2011.02.001, invited review

[2] Tunable Multifunctional Topological Insulators in Ternary Heusler Compounds, S. Chadov, X.-L. Qi, J. Kübler, G. H. Fecher, C. Felser, S.-C. Zhang, Nature Mat. 9 (2010) 541, arXiv:1003.0193

[3] Design scheme for new tetragonal multifunctional Heusler compounds for spin transfer torque applications J. Winterlik, et al. to be submitted

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**Freitag, 06.05.2011, 17 Uhr c.t.,**  
**KIT, Campus Süd,**  
**Otto-Lehmann-Hörsaal, Physik-Flachbau (Geb. 30.22).**  
**Anschließend Nachsitzung im Gastdozentenhaus „Heinrich Hertz“**