Inverse Design on an Atomic scale: Multifunctional Heusler compounds!

Información del proyecto

IDEA HEUSLER!

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Final Report Summary - IDEA HEUSLER! (Inverse Design on an Atomic scale: Multifunctional Heusler compounds!)

Heusler compounds are a remarkable and tunable class of materials with more than 1,000 members and a wide range of extraordinary multifunctionalities. An overview over the main achievement of the project “IDEA Heusler!” in the context of the recent development of the field is given in the review “Heusler 4.0” (Wollmann et al., Annual Reviews in Materials Research, Vol. 47, 2017, arXiv:1612.05947).

Magnetic Heusler compounds have a high potential for multiple applications such as spintronics, multiferroics, spin calorics and rare earth free hard magnets. Precondition for an inverse design of this class of materials is the understanding of Heusler compounds. The electronic properties of Co2-Heusler compounds are already well understood. An important highlight was the proof of a high spin polarization in Co2MnSi thin films by “in situ” spin polarized photoemission in collaboration with the Kläui team in Mainz (Nat. Com 2014). Recently, the Mn2-Heusler compounds came to the focus of many research groups, initiated by our prediction of Mn3-xGa as a potential electrode for spin transfer torque applications fulfilling all requirements for STT-RAM. Many new tetragonal Heusler compounds Mn2YZ were synthesized as
bulk materials and thin films. Despite from a high magnetic anisotropy, several new important properties were discovered. Basis for these inventions are the general "guidelines for understanding cubic and tetragonal" manganese-rich Heusler compounds (PRB 90, 214420; PRB 92, 064417). In Mn2RhSn (PRL 113, 087203) we discovered the first Heusler compound, with noncollinear magnetism, in Mn2.5PtGa a giant exchange bias (Nat. Mat. 14, 679), and Mn2CoAl to be a spin gapless magnetic semiconductor (PRL 110, 100401). Noncollinear room temperature antiferromagnetism was found in Pt2MnGa (Nat. Com. 7, 12671). All these properties were found via inverse design. Via symmetry breaking and generating of a high spin orbit coupling, a Dzyaloshinskii-Moriya interaction was induced in these Mn2-Heusler compounds with 4d and 5d elements. A topological Hall effect in Mn2RhSn (New J. Phys. 18, 85007) thin films grown in our sputtering system are the consequence. Anti-Skyrmions at room temperatures were found in Mn1.5Pt0.5Sn (arXiv:1703.01017). The tunability of Heusler compounds will enable us to further design materials showing antiferromagnetic Skyrmions in low fields and at room temperature, important for STT applications and the by Parkin proposed race-track memory. Giant Anomalous Hall effects including the corresponding anomalous Nernst effect can be tuned by the Berry curvature in Co2YZ Heusler compounds as well as in Mn2YZ Heusler compounds.

The second area of intense research are semiconducting Heusler compounds. Highlight is our work on topological Heusler compounds. First films are prepared in our sputtering systems and will be used for devices in a next step. Single crystals of topological Heusler compounds REPtBi were successfully grown. All topological Heusler compounds show ultra-high mobilities, anti-localization effects and superconductivity with non-magnetic rare earth atoms. Weyl metals, magnetically induced, are found in magnetic REPtBi compounds (arXiv:1604.01641; , Nat. Mat. 15, 1149). The topological surface state was observed in LnPtBi (Nat. Com. 7, 12924). Single crystals of superconducting Heuslers were investigated by the group of Kapitulnik, Stanford University. They found evidence for non-conventional superconductivity in agreement with a non-centro symmetric structure. These single crystals were used for nano-SQUID’s consisting of TI superconductors and normal superconductors with the goal to search for Majorana quasiparticles in collaboration with Reiss, Bielefeld. In the area of thermoelectric Heusler compounds we achieved a ZT >1 in a p-type Heusler compound based on CoTiSb (J. Mat. Chem. C 3, 10409). This is the highest value reported for this class of materials.

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