Geometry and disorder effect on the magnetic and electronic structure of Heusler compounds with high polarization

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Introduction:

A new class of systems with high polarization has attracted considerable attention in the last few years, primarily due to potential applications in the emerging field of spin-based electronics (spintronics). Promising candidates for these materials are the half-metallic Heusler compounds, which are characterized by the presence of a band gap in only one spin direction and by metallic properties in the other spin direction. High spin polarization at surfaces and interfaces is a key component for transport of information using the spin degree of freedom of the electron. Unfortunately, the physics and chemistry of surfaces can reduce this spin polarization through chemical inhomogeneity, strain or surface reconstruction. In many cases it is exceedingly difficult to fabricate a sample with perfectly 100% polarization.

Aim and methods:

The main purpose of research is to investigate the effects of geometry and disorder on electronic structure and magnetic properties on based on density-functional theory calculations. The polarization of some bulk materials will be computed using band structure calculations for the equivalent disordered system with a few % of antisite defects. Energetically prefered surface reconstruction will be studied for half-metallic Heusler compounds with 100% spin-polarization. The electronic structure, lattice dynamics and magnetic properties of selected half-metallic systems will be investigated. The calculations will be performed by using both: commercial (VASP) and open-source (Quantum-Espresso) codes.