Physics Colloquium

Half-metallic surfaces in thin-film $Ti_2MnAl_{0.5}Sn_{0.5}$: First-principles study

Dr. Pavel Lukashev

Assistant Professor, Physics Department
University of Northern Iowa

October 10, 2018
4:00 p.m.
114 Begeman Hall

Materials exhibiting a high degree of spin polarization in electron transport are in demand for applications in spintronics – an emerging technology utilizing a spin degree of freedom in electronic devices. Room-temperature half-metals are considered ideal candidates, as they behave as an insulator for one spin channel and as a conductor for the other spin channel. In addition, for nano-size devices, one has to take into account possible modification of electronic structure in thin-film geometry, due to the potential presence of surface/interface states. In this talk, I will show results of my recent density functional calculations on inverse Heusler compound, $Ti_2MnAl_{0.5}Sn_{0.5}$, which exhibits half-metallic electronic structure in bulk geometry. It will be demonstrated that in thin-film geometry, the type of termination surface has a decisive effect on half-metallicity of this material. In particular, for four out of six possible termination configurations, energy states emerge in the minority-spin band gap, significantly reducing the spin polarization of $Ti_2MnAl_{0.5}Sn_{0.5}$. At the same time, two termination surfaces preserve half-metallic properties of this material. This result is somewhat unexpected, as most of the available literature reports reduction of the spin-polarization due to the presence of surface states. These results show that a judicious choice of the termination surface may be a crucial factor in nano-device applications.

Everyone Welcome! Refreshments Provided.