Effect of Fe substitution on structural, magnetic and electron-transport properties of half-metallic Co2TiSi

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Effect of Fe substitution on structural, magnetic and electron-transport properties of half-metallic Co$_2$TiSi

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**Background**

- Research on magnetic materials for potential applications in spin-based electronics: one of the most active fields in academia and industry.
- High degree of spin polarization – wanted in spintronics.
- Spintronics – an emerging technology utilizing a spin degree of freedom in electronic devices.
- Various mechanisms which could alter the degree of transport spin polarization, such as mechanical strain, structural disorder, temperature, termination surface/interface in thin film multilayer geometry, etc.
- Magnetic materials that conduct electrons of only one spin are called half-metals, and have a great potential in spintronic devices.

**Motivation and Methods**

- Co$_2$TiSi experimentally predicted to be half-metallic, with large band gap of ~0.6 eV.
- High degree of structural order.
- Relatively high Curie temperature (around room T).
- Heusler compounds are “easy” to work with.
- Relatively ordered structures.
- Systematic increase of magnetization with Fe concentration.
- Systematic increase of $T_c$ with Fe concentration (360K for 0% Fe, 450 K for 25% Fe, 780 K for 50% Fe, 1100K for Co$_2$FeSi).
- Systematic decrease of lattice constant with Fe concentration.
- DFT – Vienna Ab Initio Simulation Package (VASP).
- Computations performed at the Department of Physics computing facilities (20-node Beowulf cluster), UNI.

**Half-metallic Heusler alloys**

- DOS (states / eV)
- E - EF (eV)
- Magnetic moment ($\mu_B$/f.u.)
- Lattice constant (Å)

**Summary**

- Combined experimental and theoretical investigation of structural, magnetic and electronic properties of Co$_2$Ti$_{1-x}$Fe$_x$Si ($x = 0, 0.25, 0.5$) Heusler alloys.
- Fe doping increases saturation magnetization.
- Curie temperature is enhanced due to Fe substitution from 340 K for Co$_2$TiSi to 780 K for Co$_2$Ti$_{0.5}$Fe$_{0.5}$Si.
- Samples are moderately conducting and show metallic electron transport.
- DFT calculations show that Fe doped material are nearly half-metallic for $x \leq 0.5$.