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Effect of Fe substitution on structural, magnetic and electron-transport properties of half-metallic \( \text{Co}_2\text{TiSi} \)

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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

- \( \text{Co}_2\text{TiSi} \) experimentally predicted to be half-metallic, with large band gap of \(-0.6 \text{ eV}\).
- 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 \( \text{Co}_2\text{FeSi} \)).
- 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)
- Lattice constant (Å)
- Magnetic moment (\( \mu_B \) / f.u.)

Summary

- Combined experimental and theoretical investigation of structural, magnetic and electronic properties of \( \text{Co}_{2-x}\text{Fe}_x\text{TiSi} \) (\( x = 0, 0.25, 0.5 \)) Heusler alloys.
- Fe doping increases saturation magnetization.
- Curie temperature is enhanced due to Fe substitution from 340 K for \( \text{Co}_2\text{TiSi} \) to 780 K for \( \text{Co}_{2-0.5}\text{Fe}_{0.5}\text{Si} \).
- Samples are moderately conducting and show metallic electron transport.
- DFT calculations show that Fe doped material are nearly half-metallic for \( x \leq 0.5 \).