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

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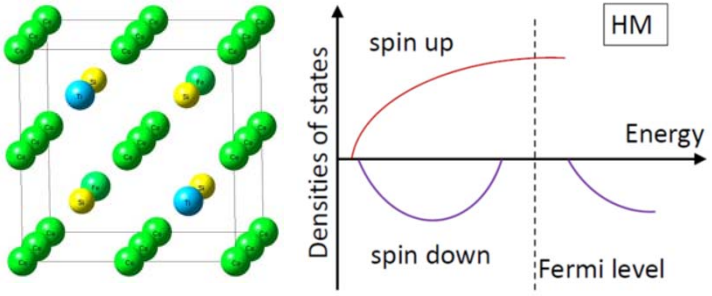
Background

- ✓ 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.

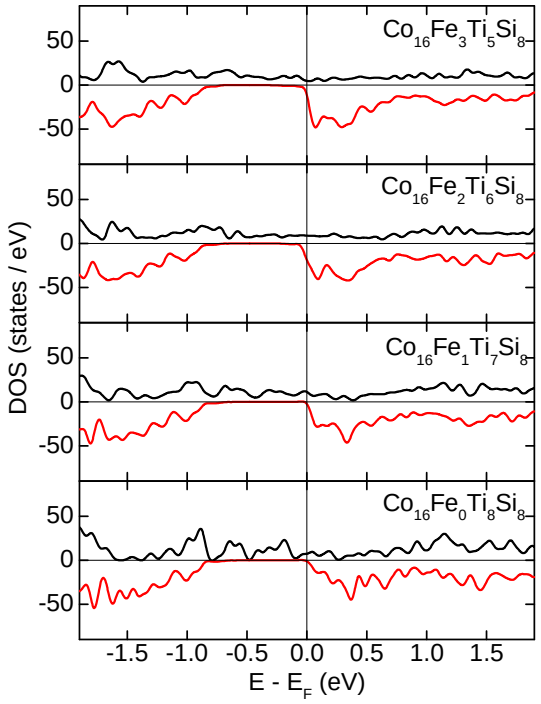
Motivation and Methods

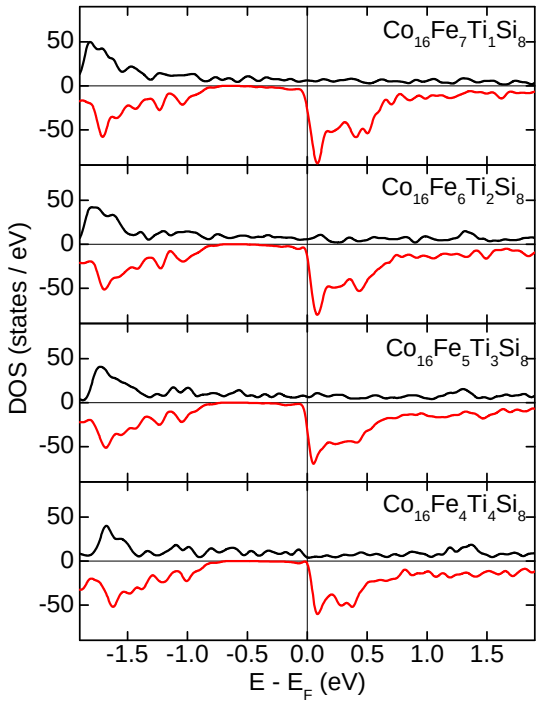
- ➢ Co_2TiSi experimentally predicted to be half-metallic, with large band gap of ~0.6 eV.
- ➢ High degree of structural order.
- ➢ Relatively high Curie temperature (around room T).
- ➢ Heusler compounds are "easy" to work with.
- ➢ Relatively ordered structures.
- ➢ Systematic increase of magnetization 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_2FeSi).
- ➢ 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.

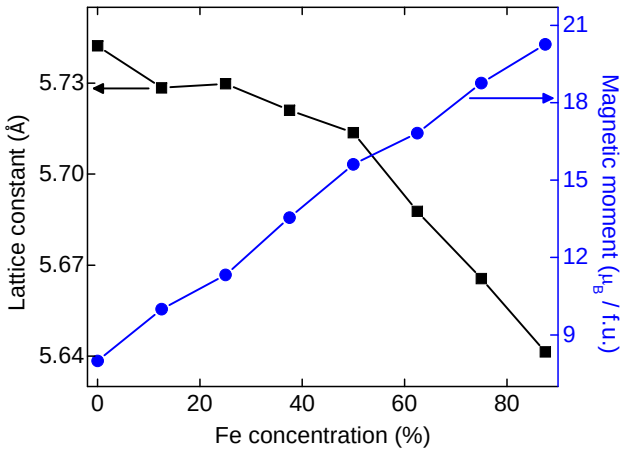
Half-metallic Heusler alloys



Electronic, magnetic, and structural properties







Summary

- ✓ Combined experimental and theoretical investigation of structural, magnetic and electronic properties of $Co_2Ti_{1-x}Fe_xSi$ (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_2TiSi to 780 K for $Co_2Ti_{0.5}Fe_{0.5}Si$.
- ✓ Samples are moderately conducting and show metallic electron transport.
- ✓ DFT calculations show that Fe doped material are nearly half-metallic for $x \leq 0.5$.
- ✓ Y. Jin, J. Waybright, P. Kharel, I. Tutic, J. Herran, P. Lukashev, S. Valloppilly, and D. J. Sellmyer, Effect of Fe substitution on the structural, magnetic and electron-transport properties of half-metallic Co_2TiSi, AIP Advances **7**, 055812 (2017).