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

Juliana Herran  
*University of Northern Iowa, herranj@uni.edu*

Parashu Kharel  
*South Dakota State University*

*See next page for additional authors*

---

Let us know how access to this document benefits you

Copyright ©2018 Juliana Herran

Follow this and additional works at: [https://scholarworks.uni.edu/rcapitol](https://scholarworks.uni.edu/rcapitol)

Part of the Atomic, Molecular and Optical Physics Commons, and the Materials Science and Engineering Commons

---

**Recommended Citation**

Herran, Juliana; Kharel, Parashu; and Lukashev, Pavel, "Effect of Fe substitution on structural, magnetic and electron-transport properties of half-metallic Co2TiSi" (2018). *Research in the Capitol*. 3.  
[https://scholarworks.uni.edu/rcapitol/2018/all/3](https://scholarworks.uni.edu/rcapitol/2018/all/3)

This Open Access Poster Presentation is brought to you for free and open access by the Conferences/Events at UNI ScholarWorks. It has been accepted for inclusion in Research in the Capitol by an authorized administrator of UNI ScholarWorks. For more information, please contact scholarworks@uni.edu.
Author
Juliana Herran, Parashu Kharel, and Pavel Lukashev

This open access poster presentation is available at UNI ScholarWorks: https://scholarworks.uni.edu/rcapitol/2018/all/3
Effect of Fe substitution on structural, magnetic and electron-transport properties of half-metallic Co$_2$TiSi

Juliana Herran, Parashu Kharel, and Pavel Lukashev

1 Department of Chemistry and Biochemistry, University of Northern Iowa, Cedar Falls, IA 50614
2 Department of Physics, South Dakota State University, Brookings, SD 57007
3 Department of Physics, University of Northern Iowa, Cedar Falls, IA 50614

**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**

- 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 $x \leq 0.5$.