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First Principles Study of Surface States and Tetragonal Distortion in Half Metals

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Half-metallic surfaces in thin-film $Ti_2MnAl_{0.5}Sn_{0.5}$

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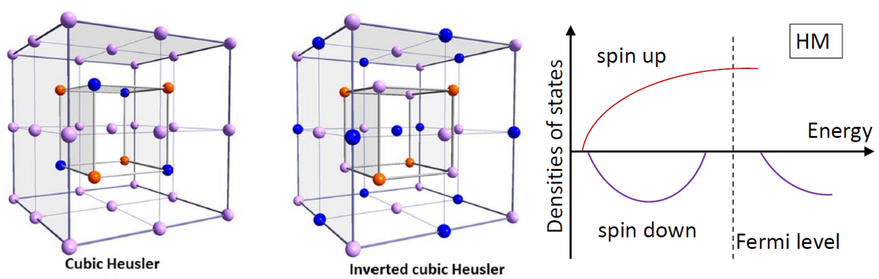
Background

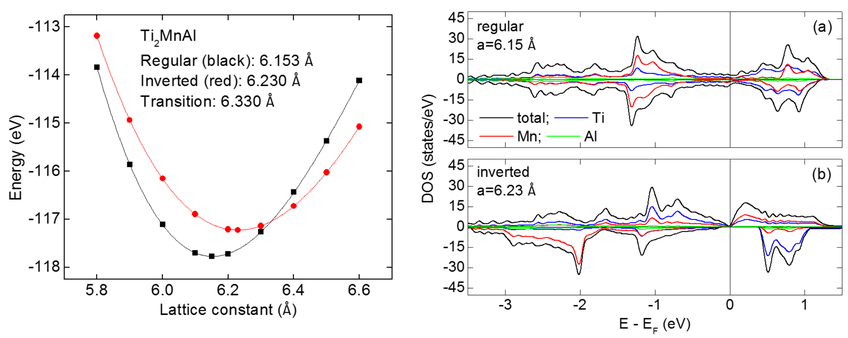
- ✓ Research on magnetic materials for potential applications in spin-based electronics: one of the most active fields in academia and industry.
- ✓ High degree of spin polarization – wanted in spintronics.
- ✓ Spintronics – an emerging technology utilizing a spin degree of freedom.
- ✓ Various mechanisms alter degree of spin polarization – 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

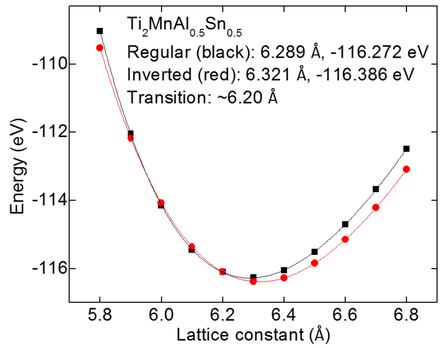
- ➢ Ideal candidate for spintronics – room temperature half-metal.
- ➢ Heusler compounds attractive because of high Curie temperature.
- ➢ $Ti_2MnAl_{0.5}Sn_{0.5}$: half-metallic electronic structure in bulk geometry.
- ➢ But is it half-metallic in thin-film geometry?
- ✓ Detrimental effect of surfaces on half-metallicity reported in the past.
- ✓ DFT – Vienna Ab Initio Simulation Package (VASP).
- ✓ Computations performed at the Department of Physics computing facilities (20-node Beowulf cluster), UNI, and at the Pittsburgh Supercomputing Center – Bridges.

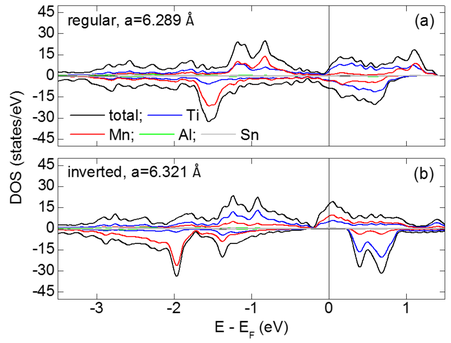
Ti_2MnAl – bulk





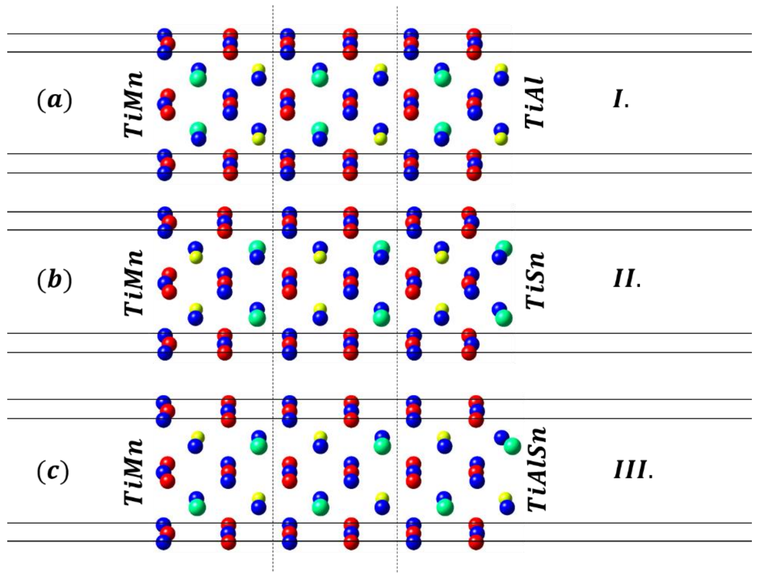
$Ti_2MnAl_{0.5}Sn_{0.5}$ – bulk half-metal

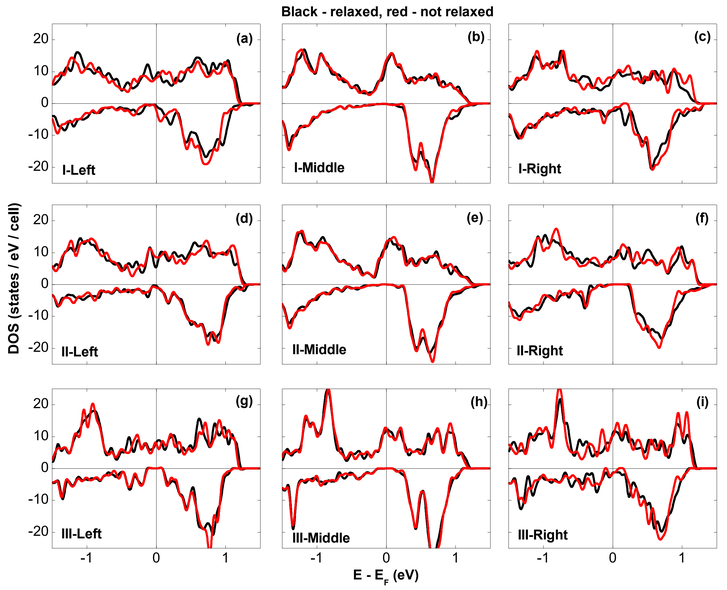




- ✓ Replacement of 50% of Al with Sn results in increase of lattice constant.
- ✓ Inverted cubic structure is ground state.
- ✓ $Ti_2MnAl_{0.5}Sn_{0.5}$ – half-metal in bulk geometry.
- ✓ Strain induced half-metallic transition,
- ✓ For applications thin films are needed.
- ✓ Is it half-metallic in thin-fil geometry?

$Ti_2MnAl_{0.5}Sn_{0.5}$: thin-film half-metal





Conclusions and References

- ✓ $Ti_2MnAl_{0.5}Sn_{0.5}$: half-metal in bulk geometry: metal for spin-up, semiconductor spin-down states.
- ✓ Six termination configurations analyzed: for 4 of them, energy states emerge in the minority-spin band gap
- ✓ Two termination surfaces preserve half-metallic properties of this material.
- ✓ Surface states in part due to Al, and its hybridization with other atoms. Atomic relaxations have negligible effect on surface HM.

- ✓ *"Half-metallic surfaces in thin-film $Ti_2MnAl_{0.5}Sn_{0.5}$", Sam Prophet, Rishabh Dalal, Parashu R Kharel, and Pavel V Lukashev, J. Phys.: Condens. Matter* ***31****, 055801 (2019).*
- ✓ *"Investigation of spin-gapless semiconductivity and half-metallicity in Ti_2MnAl-based compounds", P. Lukashev, P. Kharel, S. Gilbert, B. Staten, N. Hurley, R. Fuglsby, Y. Huh, S. Valloppilly, W. Zhang, K. Yang, R. Skomski, and D. J. Sellmyer; Appl. Phys. Lett.* ***108****, 141901 (2016).*