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

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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.
- Ti₂MnAl₀.₅Sn₀.₅: 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.

Ti₂MnAl – bulk

- Half-metallic 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.