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# Chemical Substitution Induced Half-Metallicity in CrMnSb0.5Si0.5

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# Chemical substitution induced half-metallicity in $CrMnSb_{0.5}Si_{0.5}$

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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, etc.**
- **Magnetic materials that conduct electrons of only one spin are called half-metals, and have a great potential in spintronics.**

## Computational methods and resources

**Software:**

**Density Functional calculations**

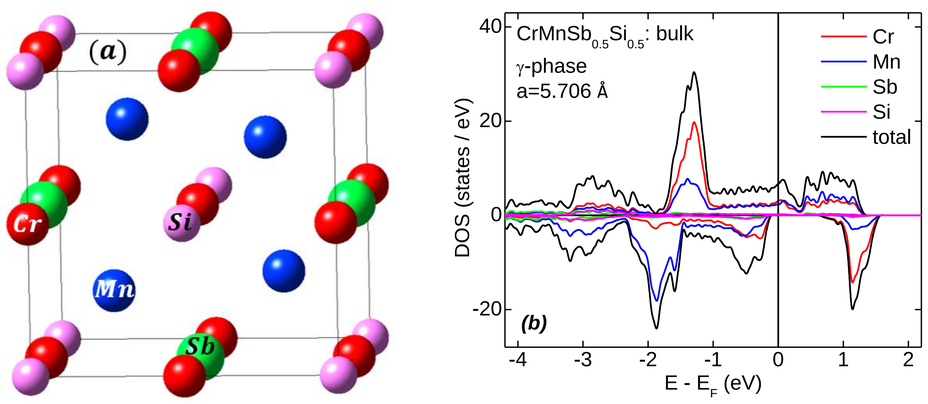
**Vienna *Ab-Initio* Simulation package (VASP)**

**Hardware:**

**Local: UNI Physics computer cluster**

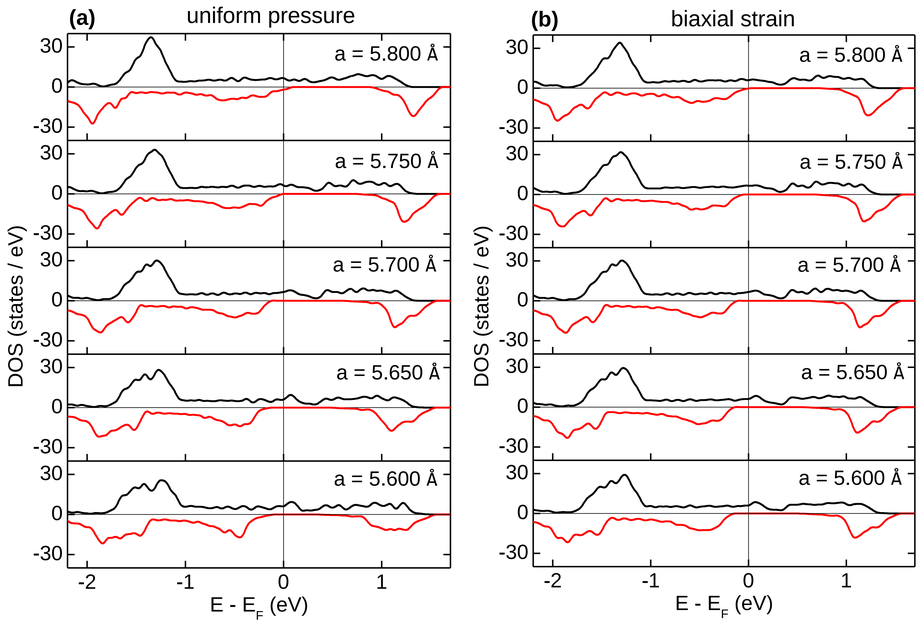
**External: Pittsburgh Supercomputing Center – Bridges 2**


## $CrMnSb_{0.5}Si_{0.5}$: crystal and electronic structures



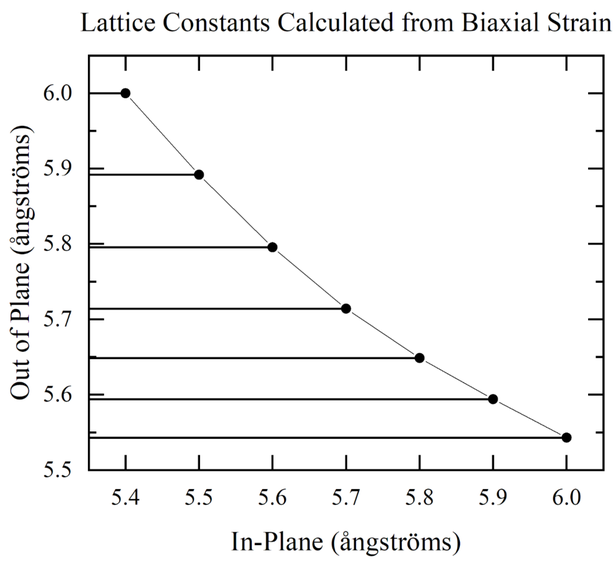

Crystal structure of $CrMnSb_{0.5}Si_{0.5}$ in $\gamma$-phase. Atoms are color-coded as indicated in the figure: Cr – red, Mn – blue, Sb – green, Si – magenta; (b) Calculated density of states of bulk $CrMnSb_{0.5}Si_{0.5}$ in $\gamma$-phase. Atomic contributions are color-coded as indicated in the figure.

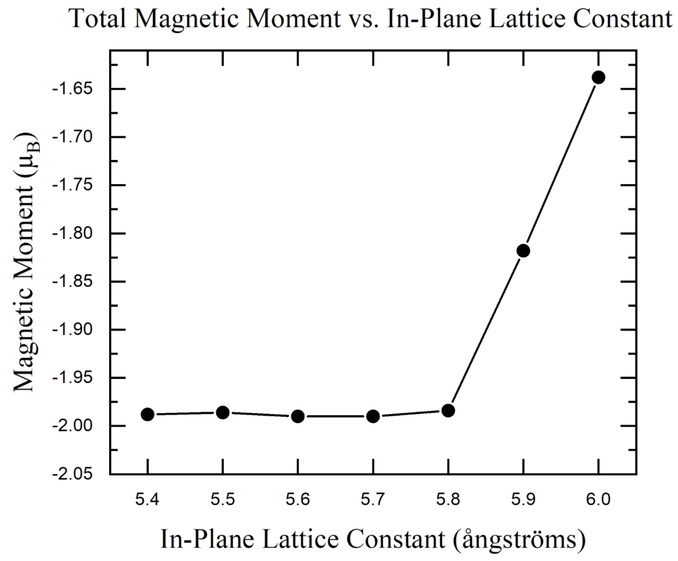
## Density of states (DOS) under pressure and strain




Calculated density of states of bulk $CrMnSb_{0.5}Si_{0.5}$ in $\gamma$-phase as a function of lattice constant, for uniform compression / expansion (a) and for biaxial strain (b). Positive and negative DOS correspond to majority- and minority- spin states, respectively. In-plane lattice parameters at which DOS is calculated are indicated in the figure.

## Magnetic moment under biaxial strain




## Summary

→ We calculated the most likely out of plane lattice constants (C values) for various in plane lattice constants (A values) of $CrMnSb_{0.5}Si_{0.5}$.

→ Using those C values, we calculated the density of states and magnetic moments of $CrMnSb_{0.5}Si_{0.5}$ across a range of A values.

→ We found a range of A values that produce a total magnetic moment of -2 $\mu_B$, as well as a density of states such that, around the Fermi energy, there are occupied states for electrons of one spin while for the opposite spin there are none.

→ Because of this, the material conducts electrons of the spin which has occupied states at Fermi level, while insulating against electrons of the other spin, a phenomenon known as half-metallicity.

## Acknowledgments

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