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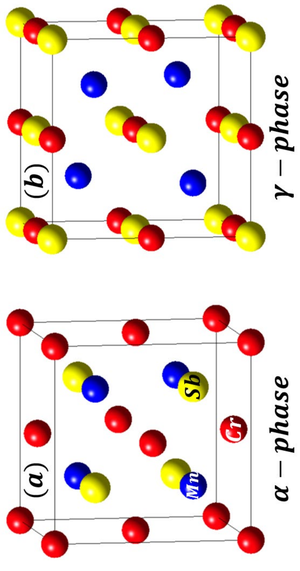
Background

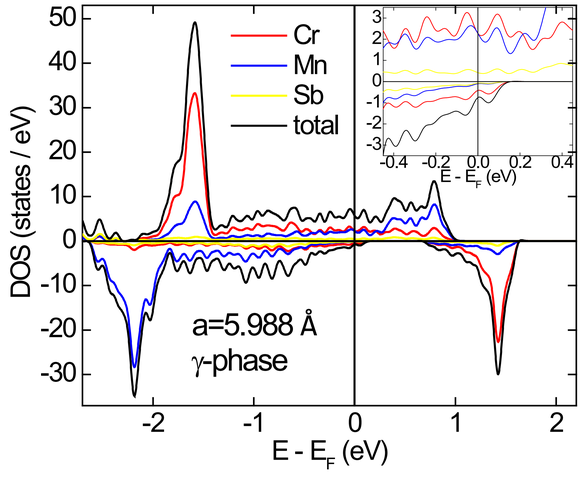
- ✓ Research on magnetic materials for potential applications in spin-based electronics: one of the most active fields in academia and industry.
- ✓ High degree of spin polarization – wanted in spintronics.
- ✓ Spintronics – an emerging technology utilizing a spin degree of freedom.
- ✓ Various mechanisms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

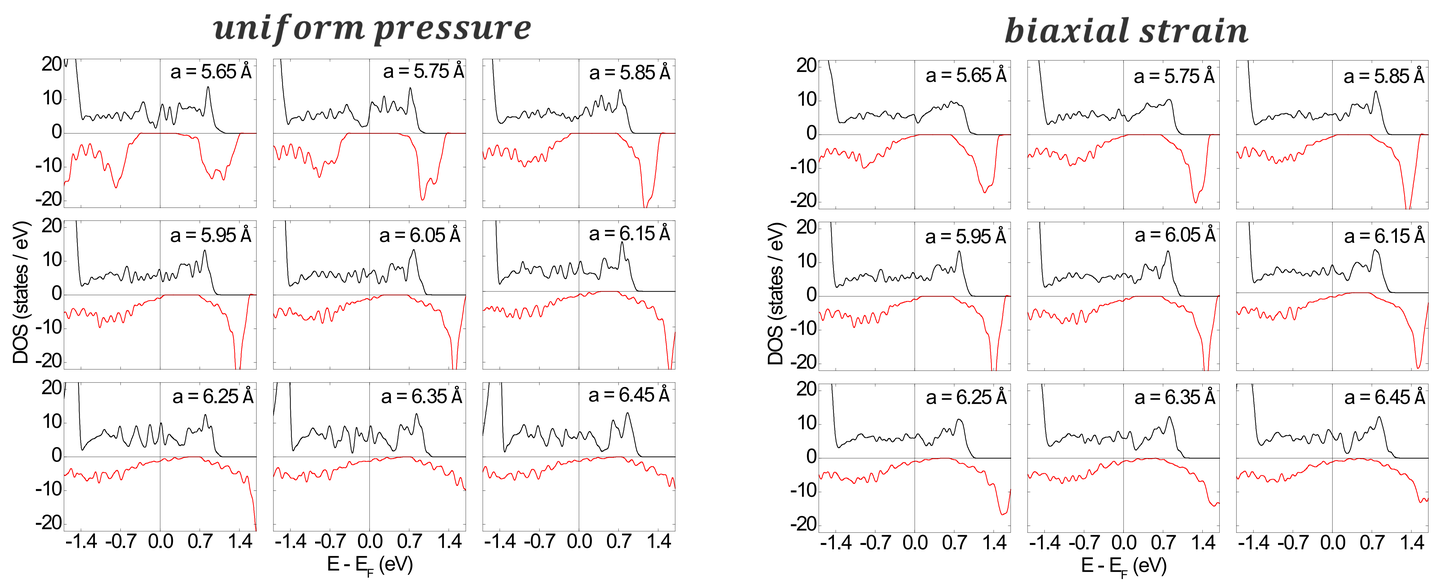
- ➢ CrMnSb and similar half-Heusler alloys may crystallize in two different phases: α-phase, and γ-phase.
- ➢ The γ-phase is energetically favorable and is nearly half-metallic.
- ➢ Can we make it truly half-metallic by external pressure / strain, or by chemical substitution?
- ➢ Epitaxial strain is more realistic scenario in thin-film applications.
- ✓ DFT (density functional theory) – Vienna Ab Initio Simulation Package (VASP).
- ✓ Computations performed at the Department of Physics computing facilities (20-node Beowulf cluster), UNI.

CrMnSb: ground state properties

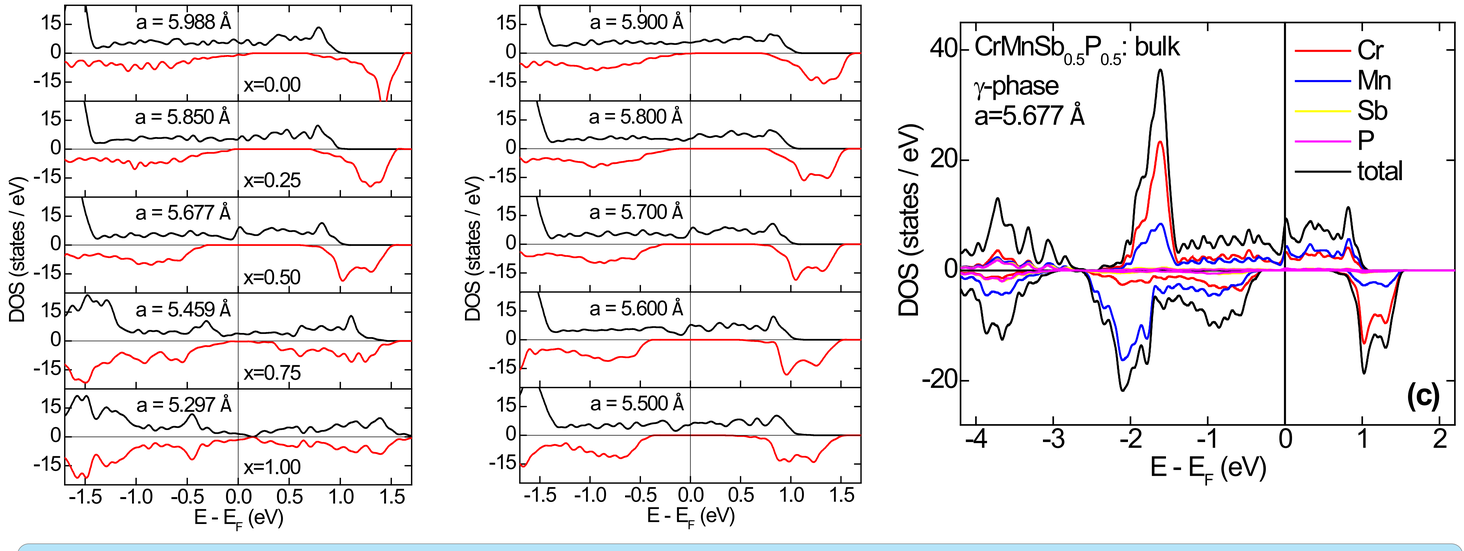




CrMnSb under pressure / strain



$CrMnSb_{0.5}P_{0.5}$: effect of chemical substitution



Conclusions and Acknowledgments

- ✓ CrMnSb is not half-metallic in ground state, despite earlier reports.
- ✓ Half-metallic transition in CrMnSb could be induced by a chemical substitution of Sb with P.
- ✓ Sb-to-P substitution results in a volume reduction of the unit cell → half-metallic transition.

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