Chemical substitution induced half-metallicity in CrMnSb(1-x)Px

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Chemical substitution induced half-metallicity in CrMnSb\(_{(1-x)}P_x\)

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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: \(\alpha\)-phase, and \(\gamma\)-phase.
- The \(\gamma\)-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**

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**CrMnSb under pressure / strain**

**uniform pressure**

**biaxial strain**

**CrMnSb\(_{0.5}P_{0.5}\): effect of chemical substitution**

- 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 \(\rightarrow\) half-metallic transition.
- This research was funded by the U.S. Department of Energy, grant number DE-SC0020564.

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**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.
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