University of Northern Iowa

UNI ScholarWorks

Summer Undergraduate Research Program (SURP) Symposium

2023 Summer Undergraduate Research Program (SURP) Symposium

Jul 28th, 11:00 AM - 1:30 PM

Electronic, magnetic, and structural properties of CoVMnSb: ab initio study

Pavel Lukashev
University of Northern Iowa

Adam Ramker
University of Northern Iowa

See next page for additional authors

Let us know how access to this document benefits you

Copyright ©2023 Pavel V. Lukashev, Adam Ramker, Brandon Schmidt, Paul M. Shand, Parashu Kharel, Vagharsh Mkhitaryan, Zhenhua Ning, and Liqin Ke

Follow this and additional works at: https://scholarworks.uni.edu/surp

Recommended Citation

Lukashev, Pavel; Ramker, Adam; Schmidt, Brandon; Shand, Paul M.; Kharel, Parashu; Mkhitaryan, Vagharsh; Ning, Zhenhua; and Ke, Liqin, "Electronic, magnetic, and structural properties of CoVMnSb: ab initio study" (2023). *Summer Undergraduate Research Program (SURP) Symposium*. 25.
https://scholarworks.uni.edu/surp/2023/all/25

This Open Access Poster Presentation is brought to you for free and open access by the CHAS Conferences/Events at UNI ScholarWorks. It has been accepted for inclusion in Summer Undergraduate Research Program (SURP) Symposium by an authorized administrator of UNI ScholarWorks. For more information, please contact scholarworks@uni.edu.

Offensive Materials Statement: Materials located in UNI ScholarWorks come from a broad range of sources and time periods. Some of these materials may contain offensive stereotypes, ideas, visuals, or language.

Author

Pavel Lukashev, Adam Ramker, Brandon Schmidt, Paul M. Shand, Parashu Kharel, Vagharsh Mkhitaryan, Zhenhua Ning, and Liqin Ke

This open access poster presentation is available at UNI ScholarWorks: https://scholarworks.uni.edu/surp/2023/all/25

Electronic, magnetic, and structural properties of CoVMnSb: ab initio study

Pavel V. Lukashev,[1] Adam Ramker,[1] Brandon Schmidt,[1] Paul M. Shand,[1] Parashu Kharel,[2]
Vagharsh Mkhitaryan,[3] Zhenhua Ning,[3] Liqin Ke[3]

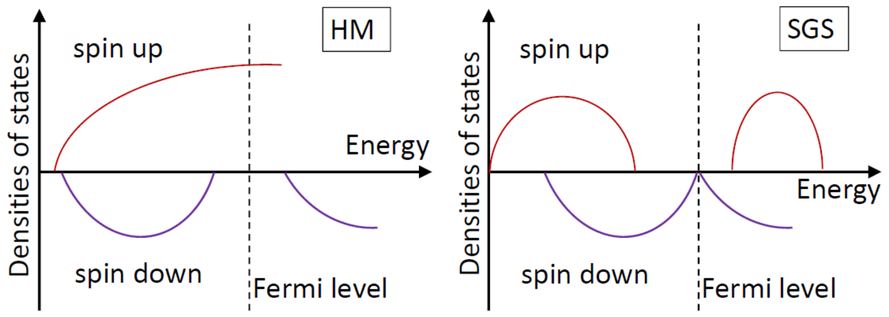
[1]*Department of Physics, University of Northern Iowa, Cedar Falls, IA 50614, USA*

[2]*Department of Physics, South Dakota State University, Brookings, SD 57007, USA*

[2]*Ames Laboratory, U.S. Department of Energy, Ames, Iowa 50011, USA*

Background

- Spin degree of freedom in electronic devices.
- Ideal candidate – room temperature half-metal.
- Heusler compounds attractive because of high Curie temperature
- Various mechanisms altering spin polarization – mechanical strain, structural disorder, temperature, termination surface/interface, etc.
- CoVMnSb: *nearly* spin gapless semiconductor.



Computational methods and resources

Software:

Density Functional calculations

Vienna *Ab-Initio* Simulation package (VASP)

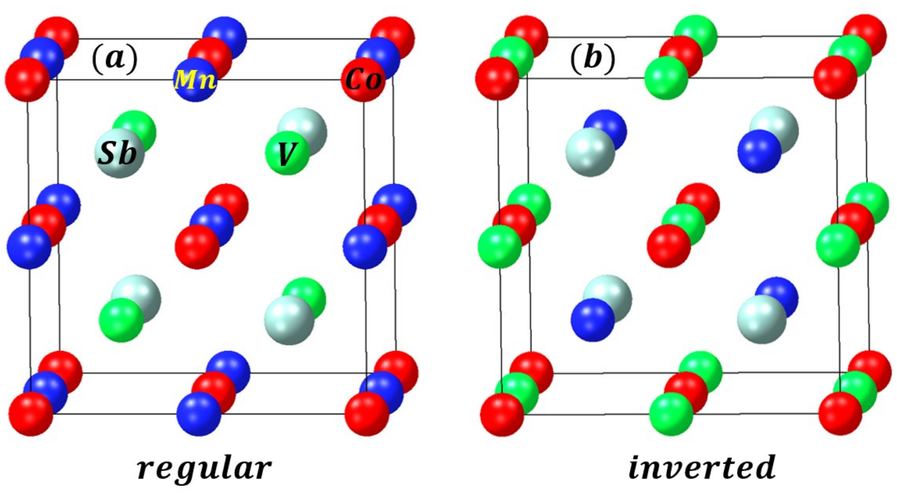
Hardware:

Local: UNI computer cluster

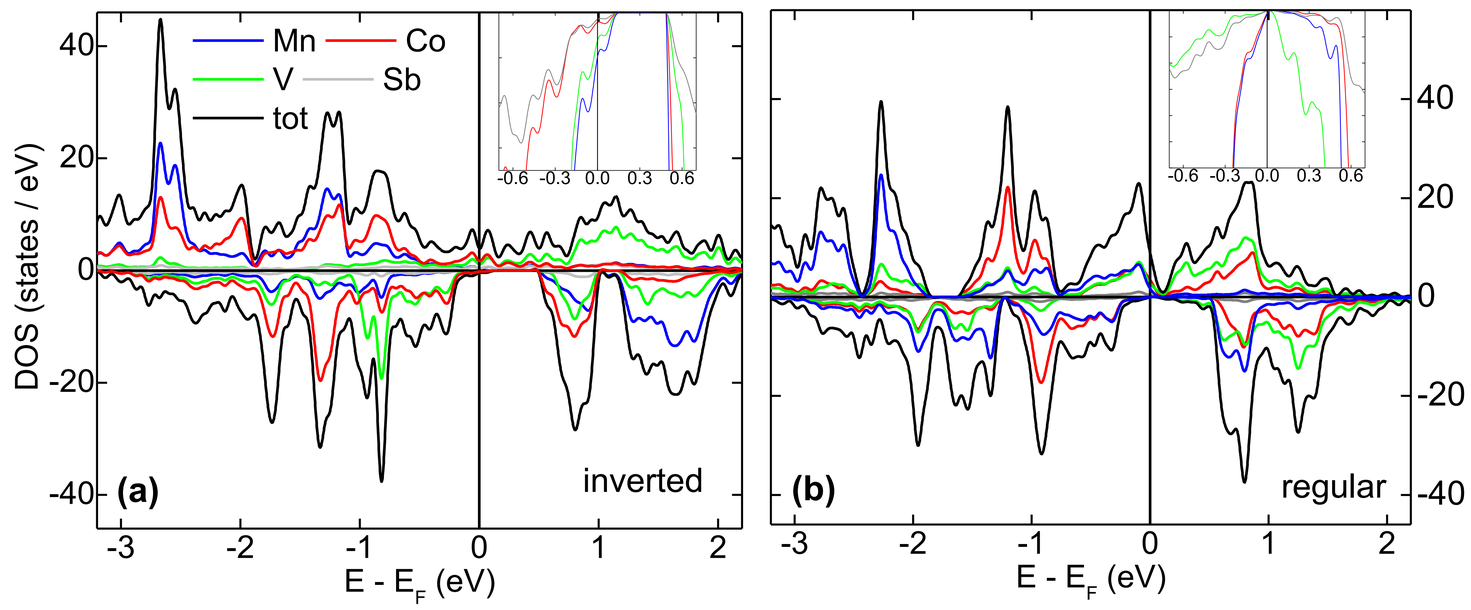
External: Pittsburgh Supercomputing Center–Bridges 2

PITTSBURGH SUPERCOMPUTING CENTER

Crystal structure



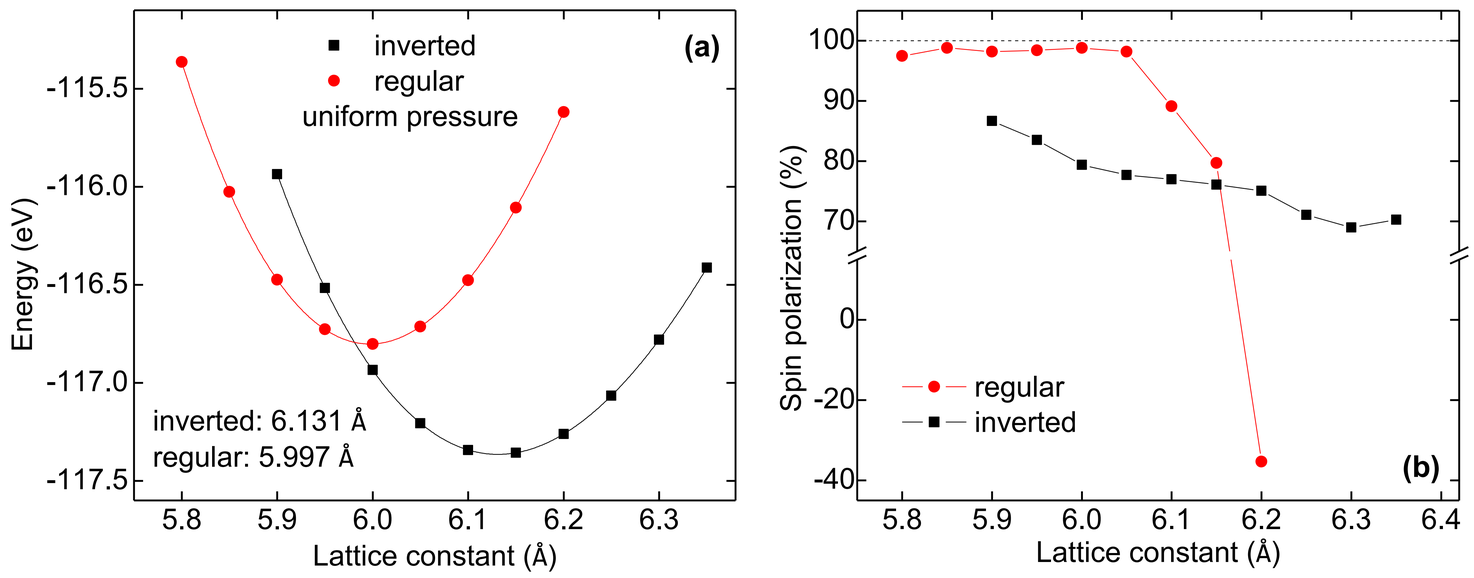
Electronic structure: density of states



Magnetic alignment

	Total (μ_B / f.u.)	Co (μ_B / atom)	Mn (μ_B / atom)	V (μ_B / atom)	Sb (μ_B / atom)
regular	2.000	1.195	0.292	0.531	-0.018
inverted	2.018	0.786	3.162	-1.735	-0.034

Mechanical pressure



Conclusions and Acknowledgments

- CoVMnSb may crystallize in two energetically close crystal structures, regular and inverted.
- Regular structure is half-metallic.
- Inverted structure has lower energy, and it exhibits reduced spin-polarization of around 80%.
- Despite having energy gap in the minority-spin channel close to the Fermi level, the inverted phase does not exhibit a half-metallic transition, e.g. under external mechanical strain.
- Instead, the half-metallic transition in CoVMnSb may be induced by a hydrostatic pressure.
- In practice, this reduction may be achieved by atomic substitutions.
- Our calculations indicated that $CoVMnSb_{0.75}Si_{0.25}$ exhibits ground state half-metallicity in a considerable range of lattice parameters.

- This research is supported by the *National Science Foundation* (NSF) under Grant Numbers 2003828 and 2003856 via DMR and EPSCoR.