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First-principles study of V(1+x)S(2-x) monolayer

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Recommended Citation

Ramker, Adam; O'Leary, Evan; and Lukashev, Pavel, "First-principles study of V(1+x)S(2-x) monolayer" (2020). *Summer Undergraduate Research Program (SURP) Symposium*. 1.
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First-principles study of $V_{(1+x)}S_{(2-x)}$ monolayer

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Background

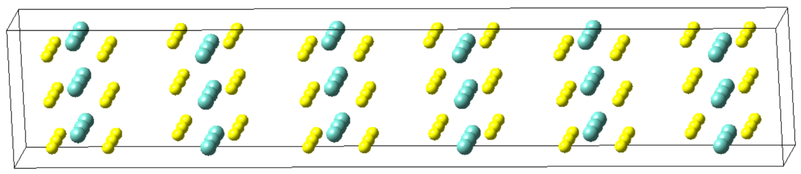
- ✓ Layered crystals are two-dimensional materials characterized by van der Waals coupling between layers.
- ✓ The two-dimensional character results in a variety of novel electronic and magnetic properties.
- ✓ The properties of these materials can be tuned by changing their chemical composition (e.g. by intercalation, or atomic substitution).
- ✓ These systems are attractive for various applications in condensed matter physics and materials science (flexible electronics, lithium-ion batteries, sensors, etc.).

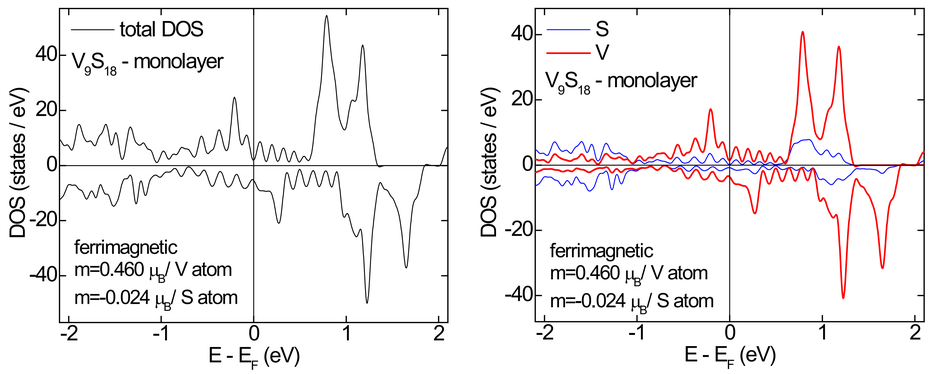
Motivation and Methods

- ➢ VS_2: 2D weakly ferromagnetic metal.
- ➢ Different crystal symmetries have been reported.
- ➢ Possible magnetic transitions in non-stoichiometric cells.
- ➢ Tuning of electronic and magnetic structure by chemical substitution.
- ➢ Potential applications in lithium-ion batteries.
- ✓ Density Functional Theory (DFT) calculations.
- ✓ Vienna Ab Initio Simulation Package (VASP).
- ✓ Computations performed at the Department of Physics computing facilities (20-node Beowulf cluster), UNI.

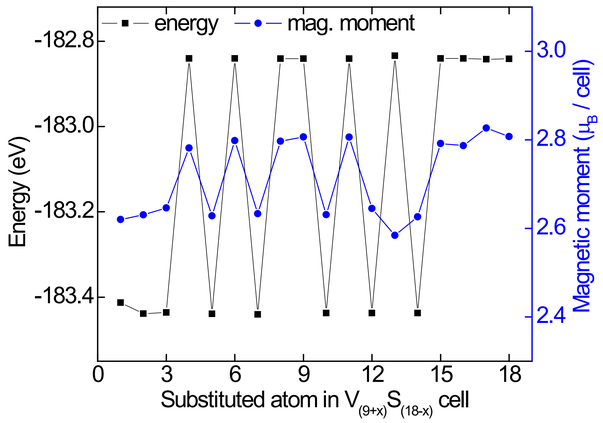
VS_2 monolayer: magnetic and electronic structure

side view: bulk

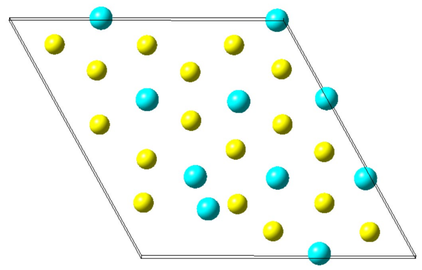




$V_{(1+x)}S_{(2-x)}$: ferrimagnetic transition

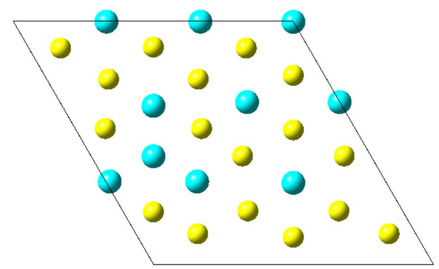


Replace 2: top view

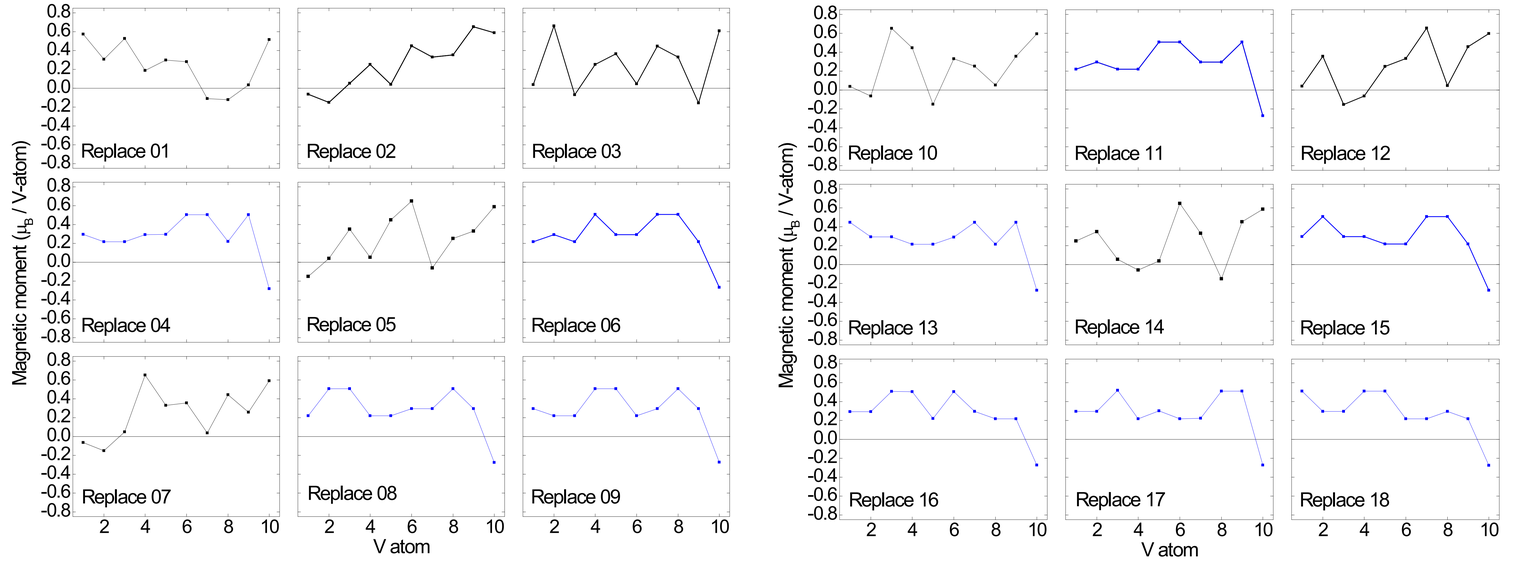


Lower energy state

Replace 4: top view



Higher energy state



Conclusions and Acknowledgments

- ✓ VS_2: weakly ferromagnetic metal in the ground state.
- ✓ Ferrimagnetic transition in non-stoichiometric $V_{(1+x)}S_{(2-x)}$.
- ✓ Two energetically close magnetic states: ferromagnetic, and ferrimagnetic.
- ✓ Lower energy state is more disordered.
- ✓ Higher energy state nearly retains the hexagonal symmetry.
- ✓ Experimental confirmation is needed.
- ✓ This research was funded by the U.S. Department of Energy, grant number DE-SC0020334.