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

Adam Ramker
University of Northern Iowa

Evan O’Leary
University of Northern Iowa

See next page for additional authors
Author
Adam Ramker, Evan O’Leary, and Pavel Lukashev

This open access presentation is available at UNI ScholarWorks: https://scholarworks.uni.edu/surp/2020/all/1
First-principles study of $V_{(1+x)}S_{(2-x)}$ monolayer

Adam Ramker,1 Evan O’Leary,1 Pavel Lukashev1

1 Department of Physics, University of Northern Iowa, Cedar Falls, IA 50614

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

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.