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

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## Background

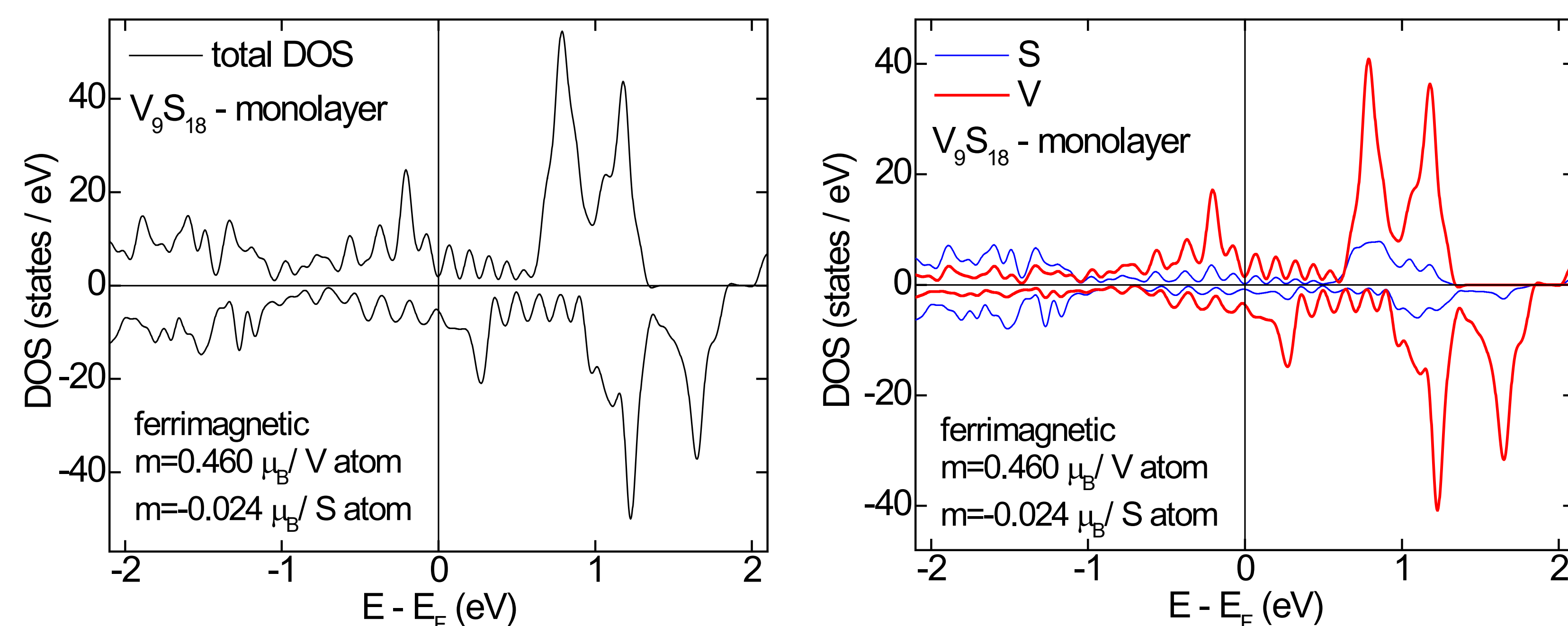
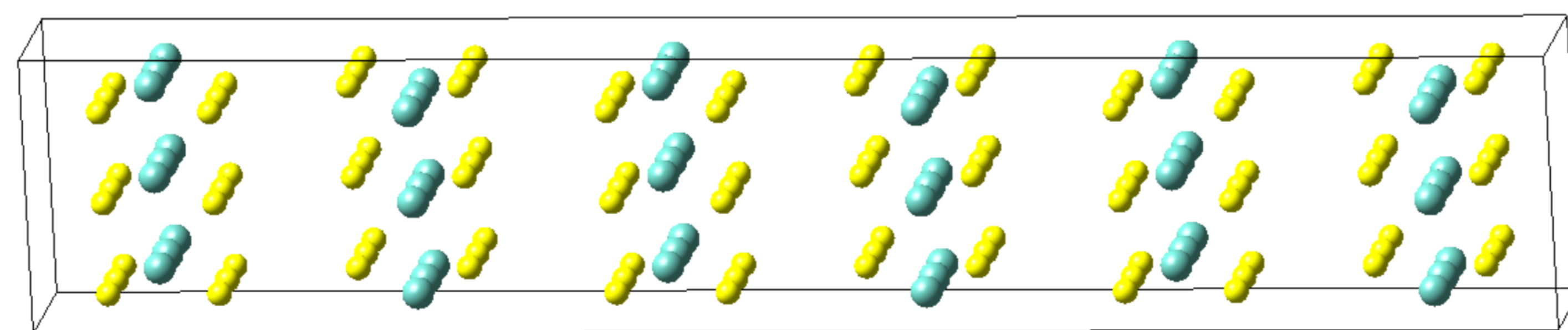
- ✓ Layered crystals are two-dimensional materials characterized by van der Waals coupling between layers.
- ✓ The two-dimensional character results in a variety of novel electronic and magnetic properties.
- ✓ The properties of these materials can be tuned by changing their chemical composition (e.g. 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

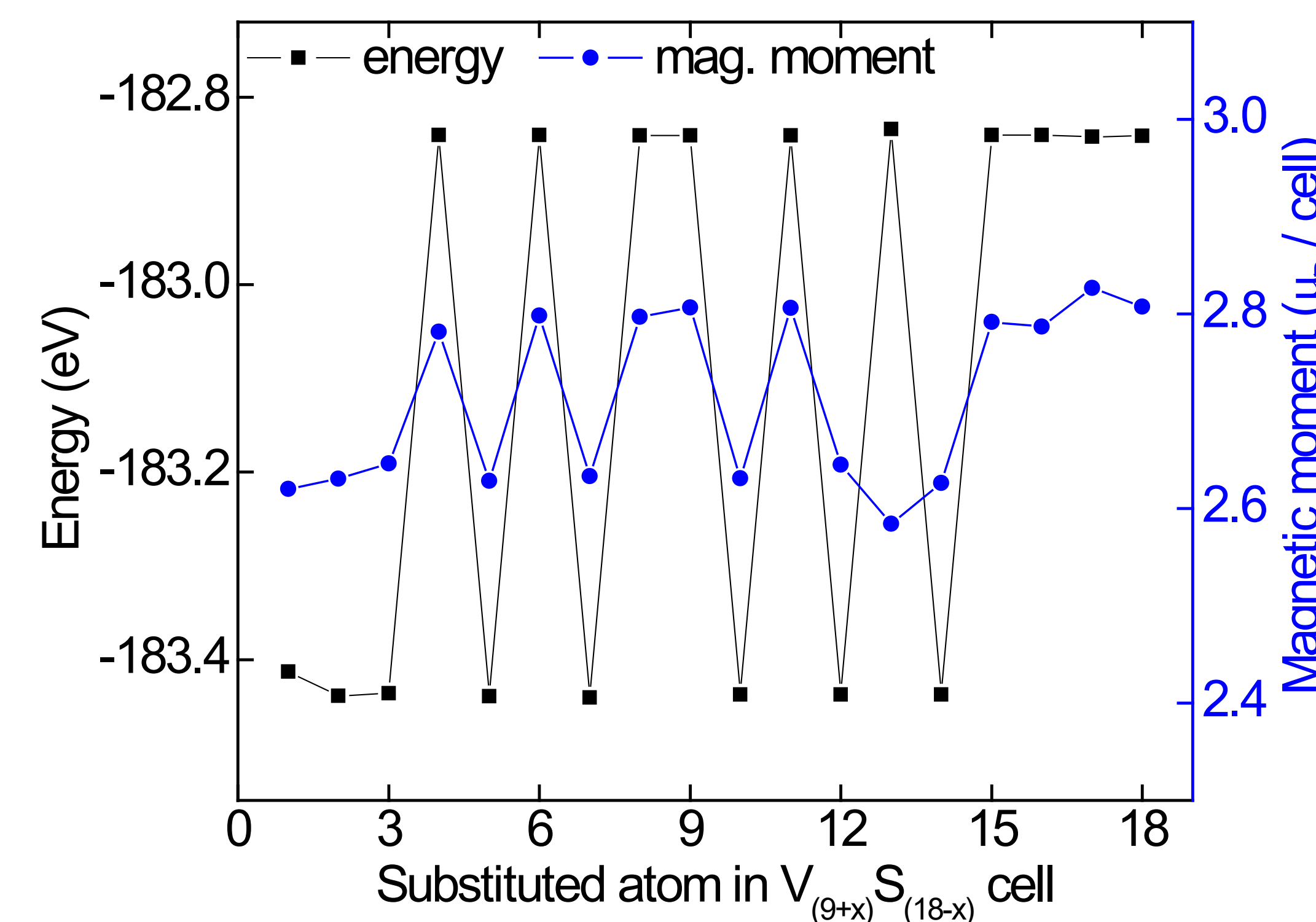
- $VS_2$ : 2D weakly ferromagnetic metal.
- Different crystal symmetries have been reported.
- Possible magnetic transitions in non-stoichiometric cells.
- Tuning of electronic and magnetic structure by chemical substitution.
- Potential applications in lithium-ion batteries.
- ✓ Density Functional Theory (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

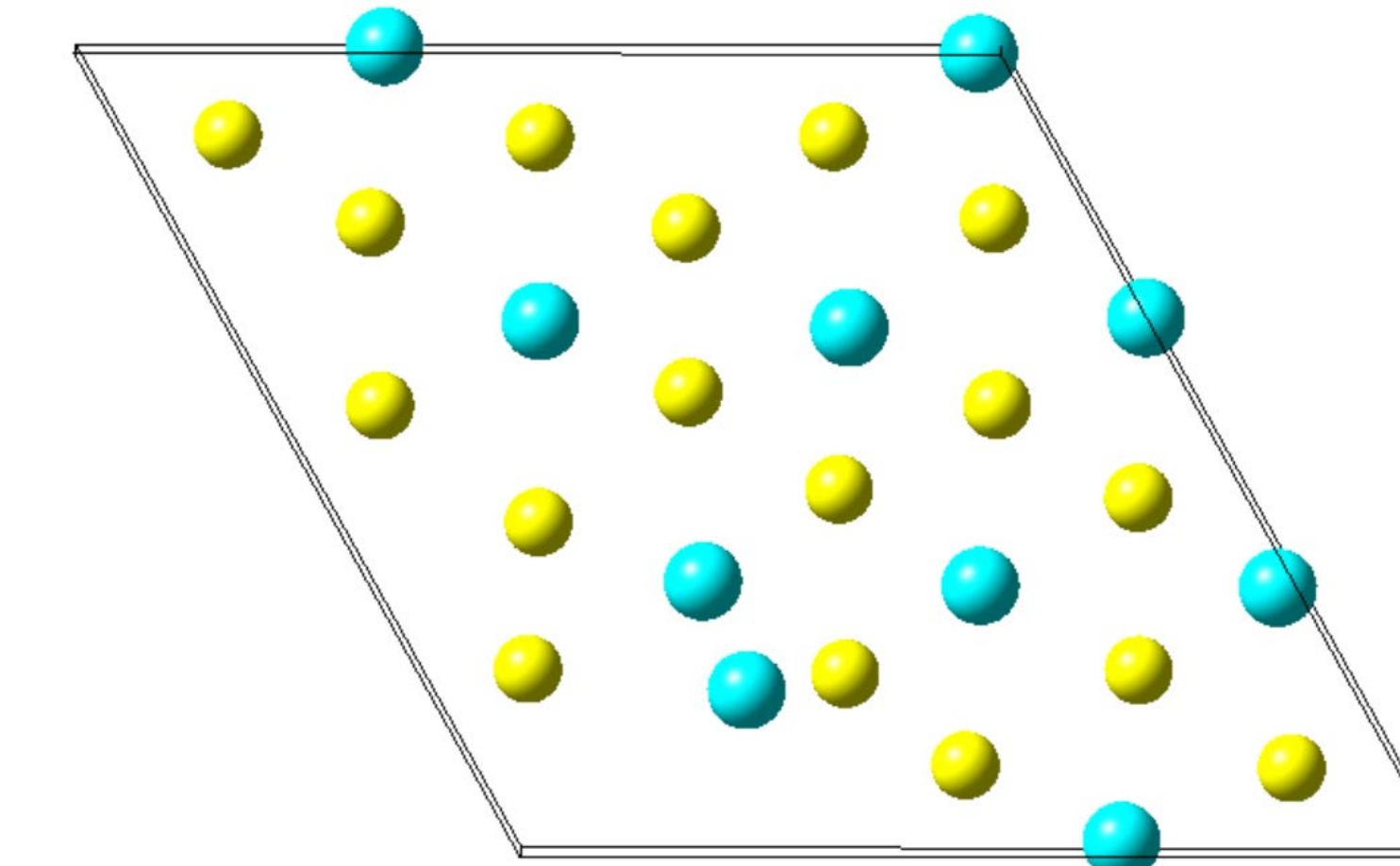
side view: bulk



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

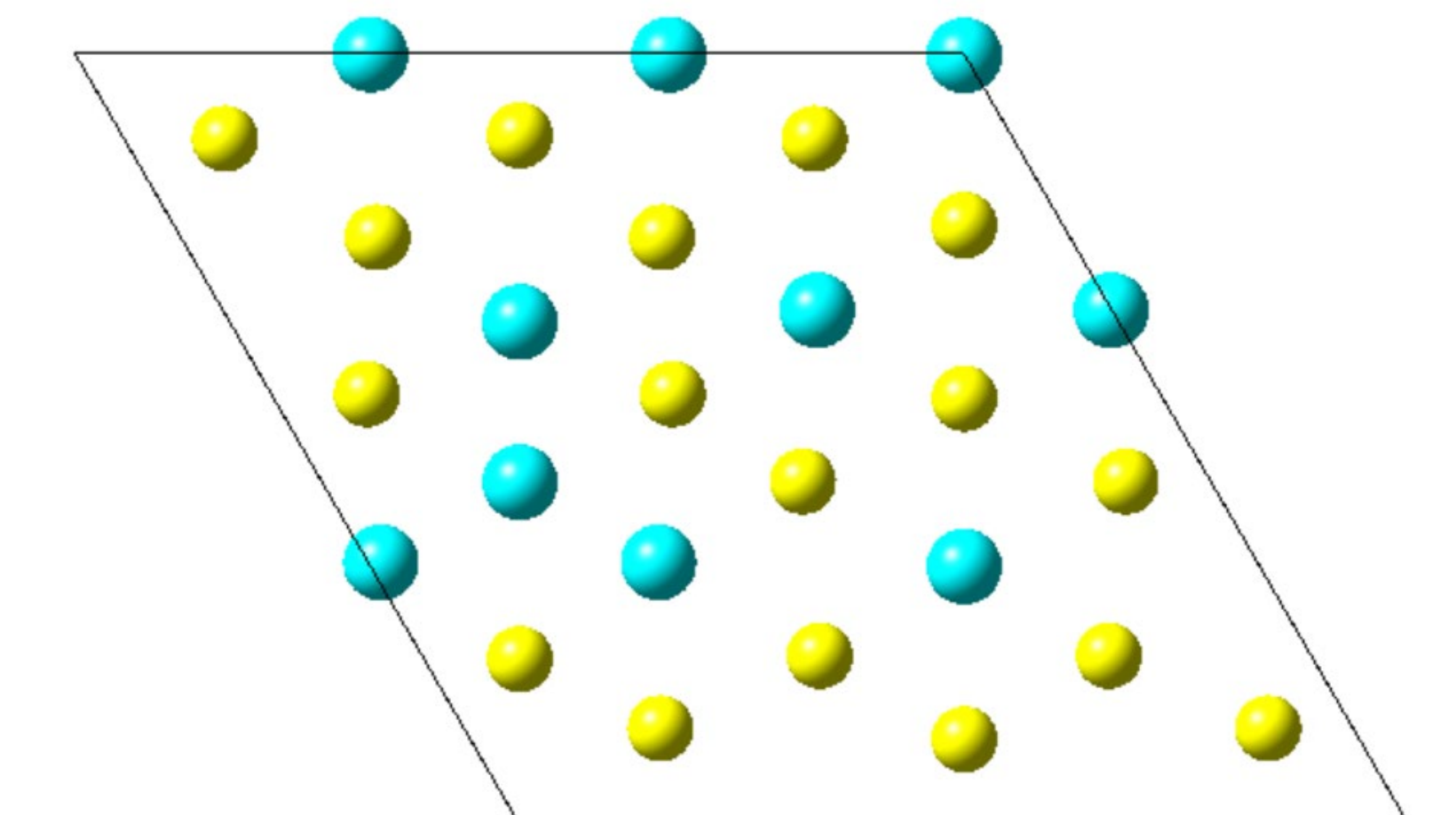


Replace 2: top view

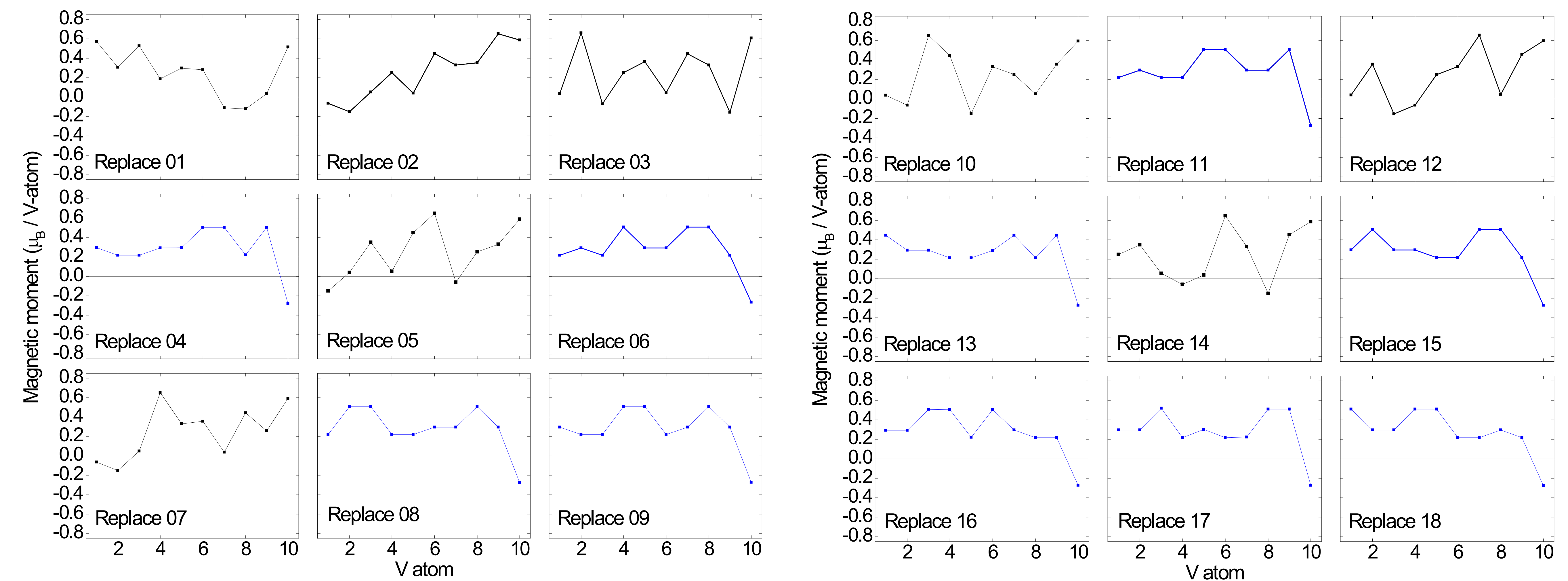


Lower energy state

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.