Introduction:

2D Transition Metal Dichalcogenides (TMDs) are atomically thin semiconductors. TMDs hold great potential for logic, memory, opto-electronic, energy harvesting, energy storage, and thermal management applications and devices. The most significant of Atomic Layer Deposition (ALD) over other methods is film conformation, low temperature processing, and the self-limiting nature of the ALD growth mechanism.

Objectives:

Screening precursors molecules for ALD is important for finding effective precursor molecules for ALD. A series of energetic calculations will be done to predict precursor properties such as bond length and strength, thermolysis energy and barrier, chelation energy, hydrolysis energy, and formation energy.

Methods:

First-principles density functional theory (DFT)
- Utilized VASP to run energetic calculations
- Computational quantum mechanical calculations were run using Boise State’s high-performance computing facilities.

Precursor Molecules:

- (MoCl₂(III) Me₂NC(NiPr)₂)
- MoF₆
- MoCl₄(V) Me₂NC(NiPr)₂
- (MoCl₂(III) Me₂NC(NiPr)₂ and Al₂O₃ surface)
- MoF₆ and Al₂O₃ surface

Conclusion and Future Work:

More calculations will be run to help determine reaction pathways and reactivity of precursors with substrate surface.

Acknowledgements: This work was supported by the National Science Foundation via the Research Experience for Undergraduates Site: Materials for Society at Boise State University (DMR 1658076).