Computational Modeling of 2D Transition Metal Dichalcogenides by Atomic Layer Deposition

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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 confomality, low temperature processing, and the self-limiting nature of the ALD growth mechanism.

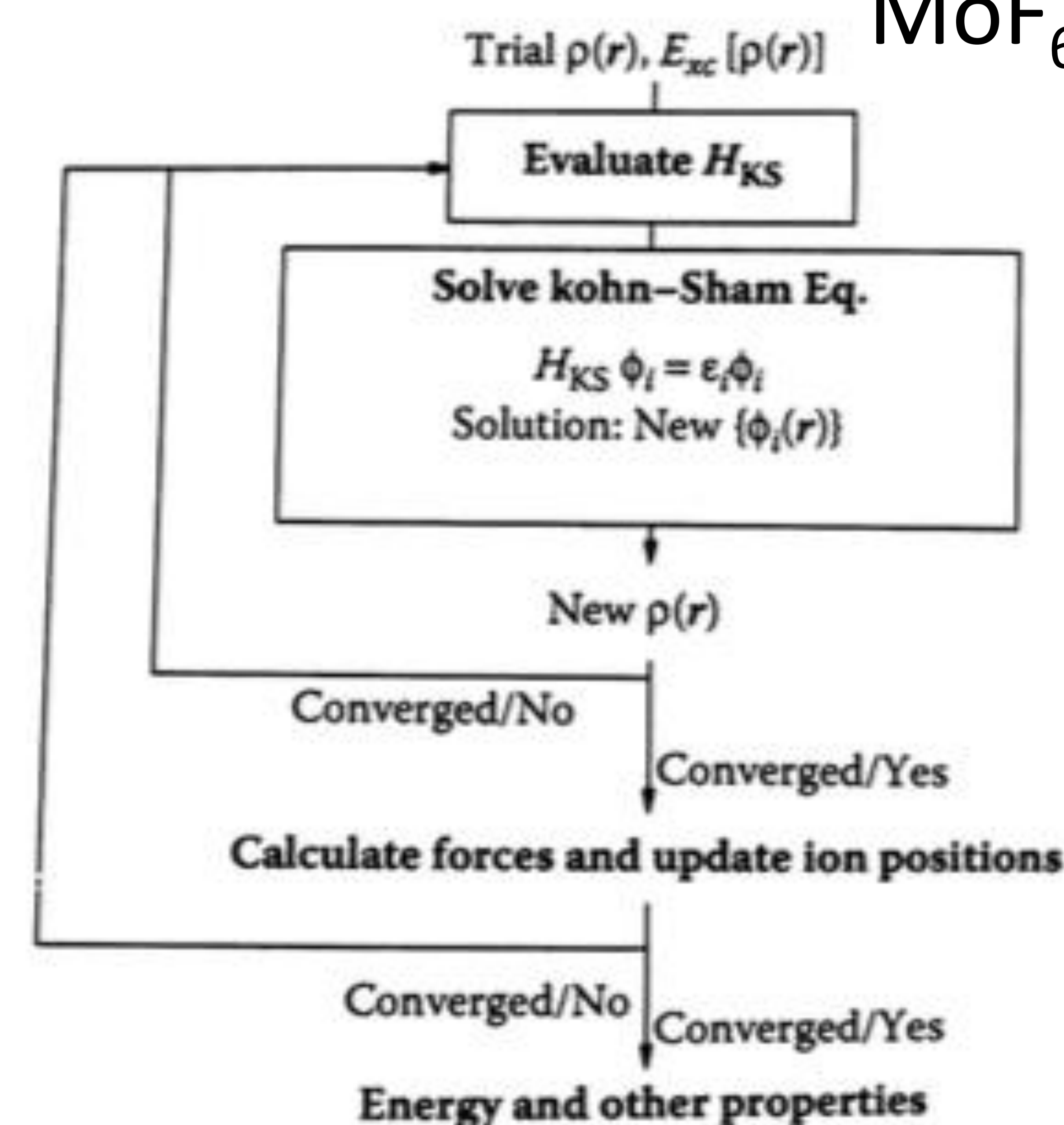
Objectives:

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:

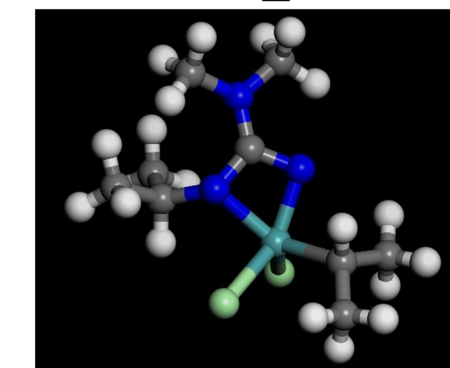
First-principles density functional theory (DFT)

- Utilized VASP to run energetic calculations
- Computational quantum mechanical calculations were run using Boise State's high-performance computing facilities .

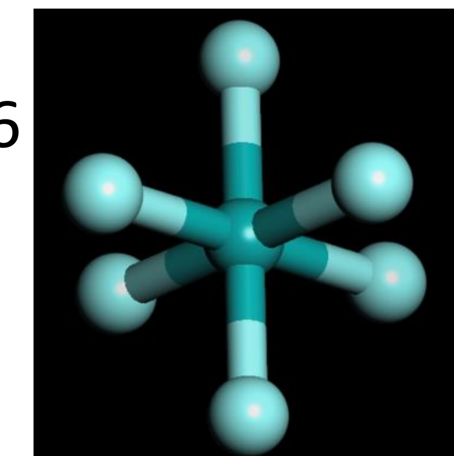


Precursor Molecules:

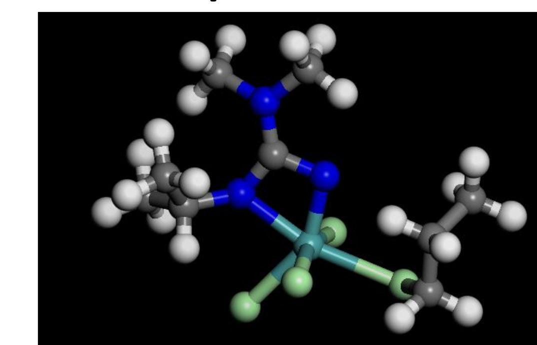
$(MoCl_2$ (III) $Me_2NC(N^iPr)_2$



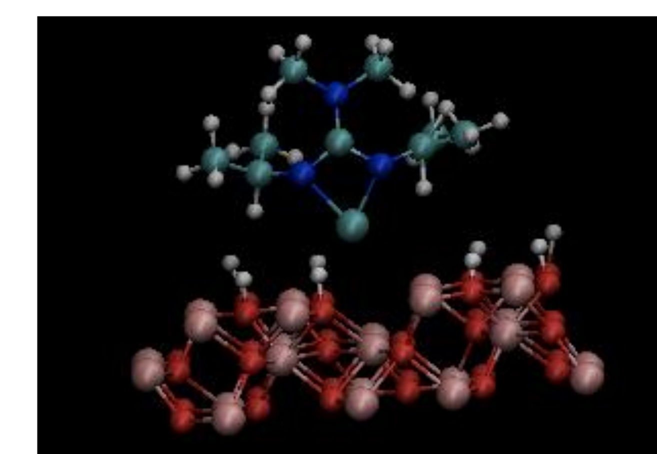
MoF_6



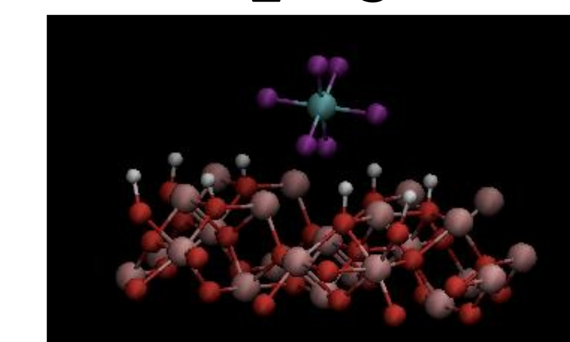
$MoCl_4$ (V) $Me_2NC(N^iPr)_2$



$(MoCl_2$ (III) $Me_2NC(N^iPr)_2$ and Al_2O_3 surface



MoF_6 and Al_2O_3 surface



Conclusion and Future Work:

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

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