Surface functionalization of monolayer MoS_2 for atomic layer deposition using gold chloride salts

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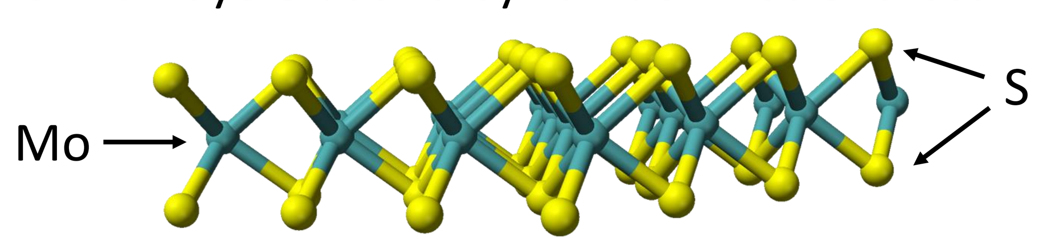
NSF ECCS 1407677

Properties of Molybdenum Disulfide

- Molybdenum disulfide (MoS_2) possesses a hexagonal, layered structure with layers bound by van der Waals forces.



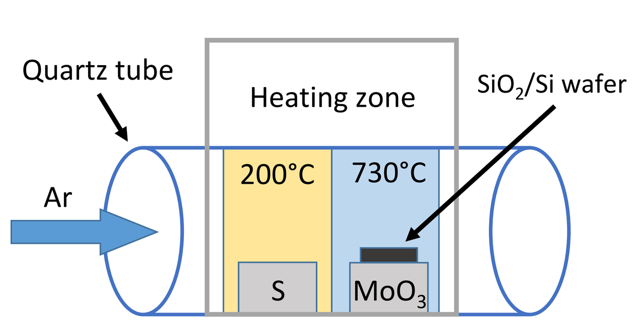
- MoS_2 possesses a direct band gap of 1.8 eV in monolayer form.
- Integration of MoS_2 with high-k dielectrics is necessary for fabrication of top-gated MOSFETs and other devices.
- The MoS_2 surface is hydrophobic and not conducive to dielectric film growth.

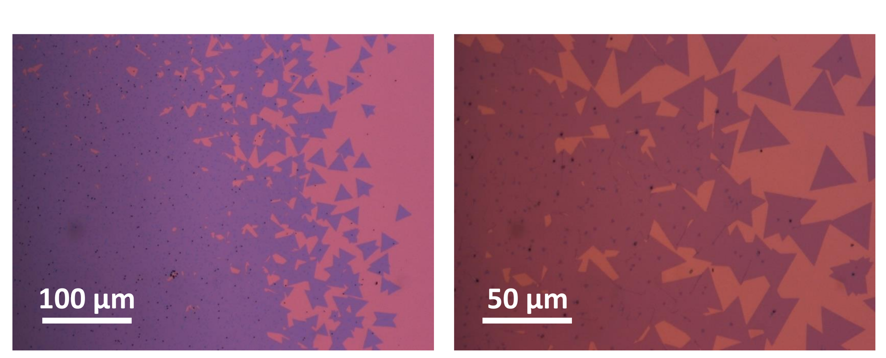
Objectives

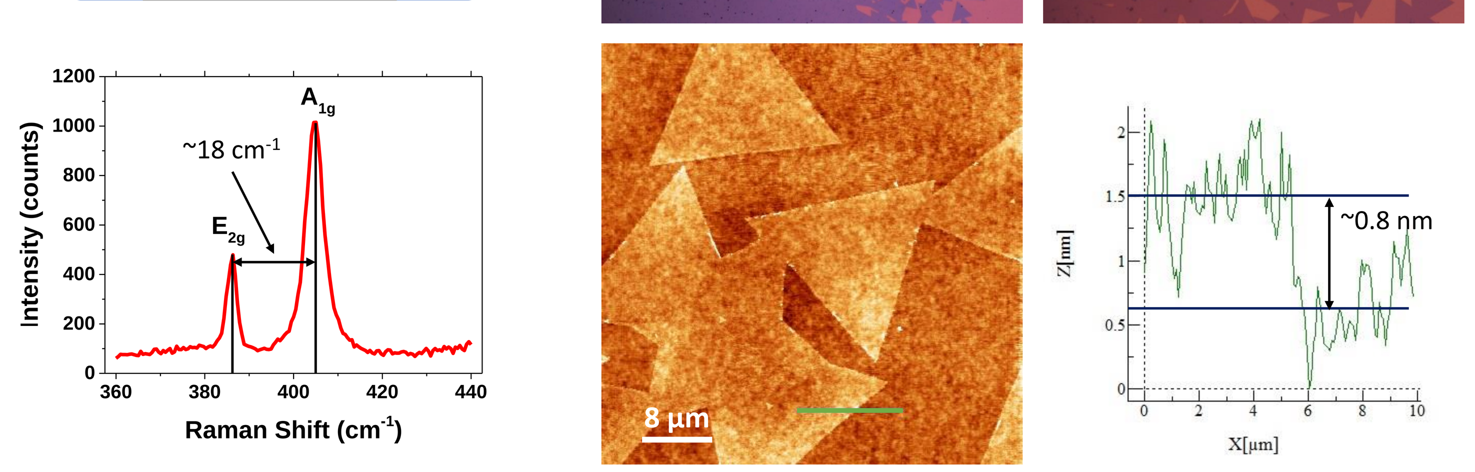
- To investigate growth mechanisms of dielectric films deposited via atomic layer deposition (ALD) on MoS_2 surfaces.
- To increase chemical reactivity of (i.e. functionalize) the MoS_2 surface.
- To deposit conformal, high-quality dielectric films on MoS_2 surfaces via ALD.

CVD-Grown MoS_2

- Molybdenum trioxide (MoO_3) and sulfur powder are used as precursors.
- Sulfur powder is evaporated upstream at 200°C.
- Downstream, 300 nm SiO_2/Si wafers are placed face down above the MoO_3 powder, heated at 730°C.
- Monolayers are confirmed via Raman spectroscopy and AFM.

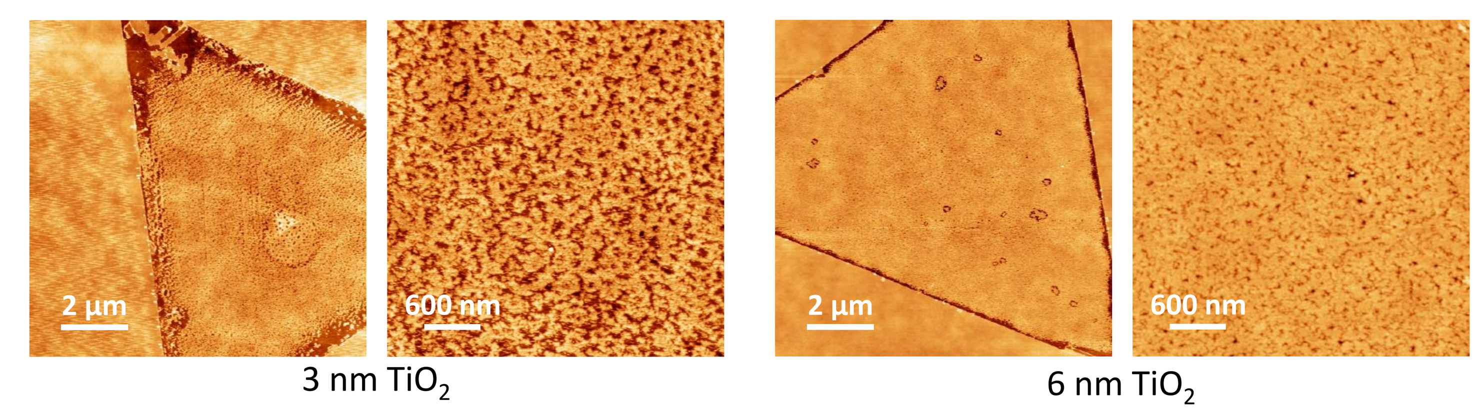






ALD on Untreated MoS_2

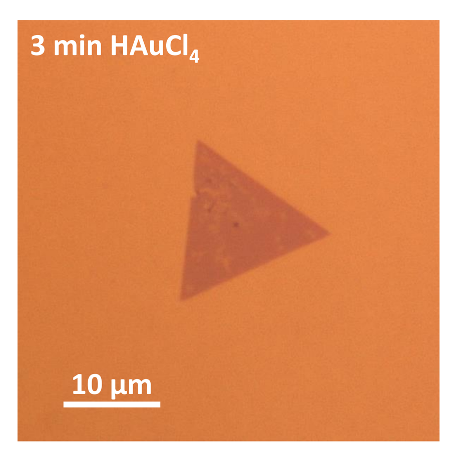
- 3 nm and 6 nm TiO_2 is grown via ALD on monolayer MoS_2 at 100°C using tetrakis(dimethylamino) titanium and water.
- At this temperature, precursor physisorption (condensation) is expected.



3 nm TiO_2 6 nm TiO_2

Surface Functionalization of MoS_2

- 5 mM $HAuCl_4$ solution was drop cast on MoS_2 monolayers for 2-3 minutes.
- Gold chloride salts are expected to bond to the sulfur surface, leaving the MoS_2 surface chlorine-terminated.
- Chlorine termination provides nucleation sites that modify the surface chemistry and seed the ALD film.



- 3 minute treatment results in reduction of $HAuCl_4$ and formation of gold nanoparticles.
- Gold nanoparticles act as a p-type dopant.
- Formation of nanoparticles may be of interest for catalysis or gas sensing.

Surface Analysis

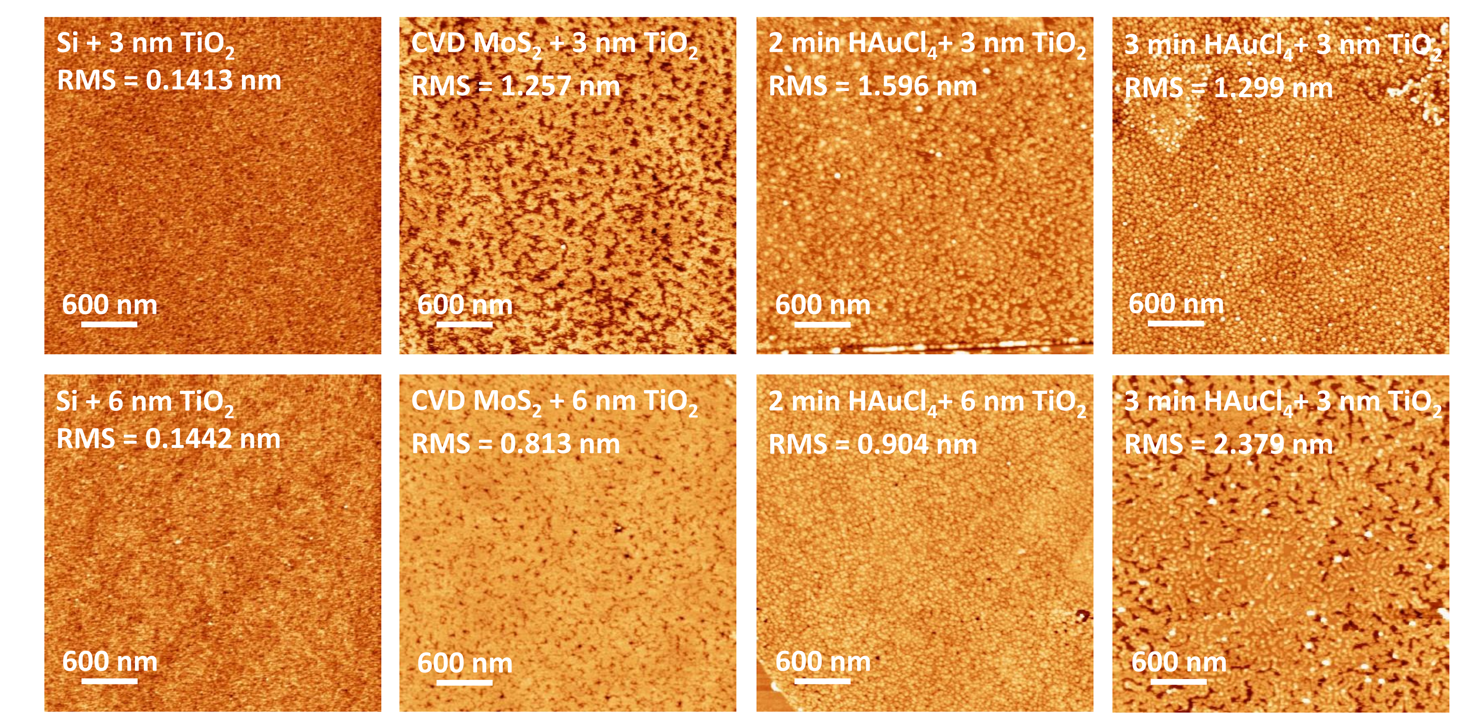
- Atomic force microscopy is used to probe the surface.
- RMS roughness: $\mathrm{RMS} = \sqrt{\frac{1}{N}\sum_i (z_i - z_{avg})^2}$
- We assume a self-affine surface such that:

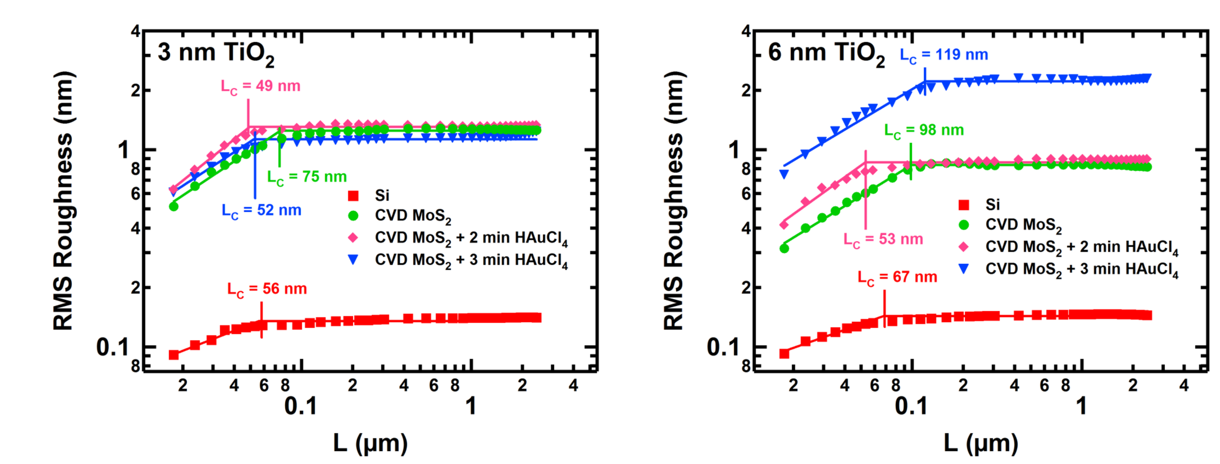
$$\mathrm{RMS} = \begin{cases} \sim L^{\alpha} & L < L_c \\ constant & L \geq L_c \end{cases}$$

- The correlation length is related to the diffusion length of precursors across the surface.

Roughness Scaling

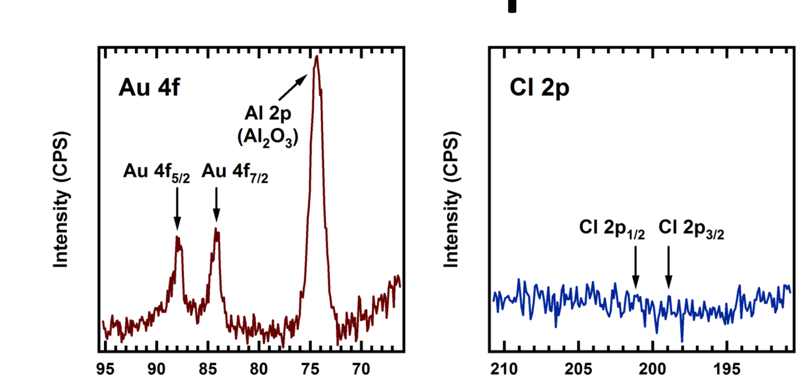
- 3 nm and 6 nm TiO_2 films are analyzed as a function of length scale.





- Gold chloride treatment alters the surface chemistry of MoS_2 and changes the way ALD precursors interact with the surface.

Compositional Analysis



- 3 nm Al_2O_3 deposited on polycrystalline* MoS_2.
- Gold remains after Al_2O_3 deposition.
- Chlorine is below XPS detection limit.

Conclusion

- Gold chloride solutions can alter the MoS_2 surface chemistry.
- Chlorine-terminated surface seeds film growth, and chlorine atoms are removed during deposition.
- Though the surface chemistry has been modified, growth of smooth dielectric films has not been achieved.

* The authors would like to acknowledge Berc Kalanyan, James Maslar, and Brent Sperling of NIST for contributing the polycrystalline MoS_2 samples used in this work.