# Thermodynamic similarities and kinetic deviations complemented by DFT: CVD of MoS2 and WS2

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Van der Waal's heterostructures have gained popularity owing to the possibility of mixing members from the large set of VdW materials with varied properties to create unique structures. Often times, the hindrance to synthesis of VdW heterostructures is difficulty in obtaining pure interface, owing to contamination during transfer of layers. We have developed a true-CVD system[1] that can be used to grow $MoS_2/WS_2$ heterostructures without needing to remove the structure from inside the reaction chamber into the ambient, in between growth, thus avoiding contamination from external environment. After having successfully achieved independent growth of $MoS_2$[2] and $WS_2$ as a first step to heterostructures, we compare and contrast thermodynamics and kinetics of growth of the two compounds. Thermodynamic modelling, based on a Gibb's free energy minimization technique, predicts similar growth trends for both systems, attested to by experiments [3]. But comparison of nucleation densities, growth rates, island sizes, and film morphology for Mo and W system paint a different picture. Experimentally required precursor flow for 2D growth of required morphology also show large deviation, caused most probably by kinetic factors. This observation is complimented by analysing kinetic effects by DFT studies of growth mechanisms. Contrast in aspects of i)binding energies to substrate surface sites, and ii) diffusion to nucleation sites are explored in DFT studies to understand variation in experimental CVD morphology of $MoS_2$ and $WS_2$.

## References

[1] V. Kranthi Kumar, Sukanya Dhar, Tanushree. H. Choudhury, S.A. Shivashankar, Srinivasan Raghavan, Nanoscale, 7, 7802 (2015)
[2] Sukanya Dhar, V. Kranthi Kumar, Tanushree. H. Choudhury, S.A. Shivashankar, Srinivasan Raghavan , Phys. Chem. Chem. Phys., 18, 8 (2016)
[3] Sukanya Dhar, Anjali Lalithambika, Kranthi Kumar V and Srinivasan Raghavan, ECS. Trans., 77, 49 (2017)

## Figures

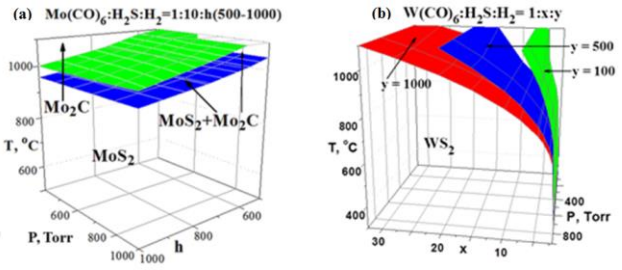


**Figure 1:** Phase stability diagrams constructed for hydrogen ambient using thermodynamic modelling showing similar trends for a) $MoS_2$ and b)$WS_2$ systems

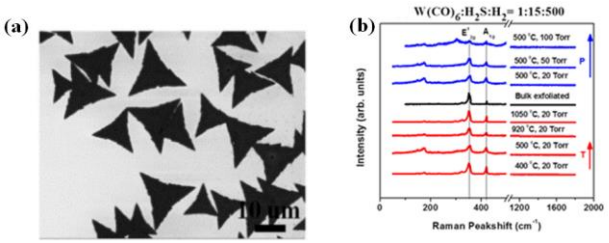


**Figure 2:** a) SEM presenting $MoS_2$ islands ~10 um, b) $WS_2$ grown under similar conditions shows no discreet morphology, but is pure $WS_2$ as predicted in Fig. 1, confirmed by Raman spectra