GRAPHENE AND 2DM VIRTUAL CONFERENCE & EXPO

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In situ and *ex situ* assessment of carbon contamination in MOCVD-grown MoS_2 thin films

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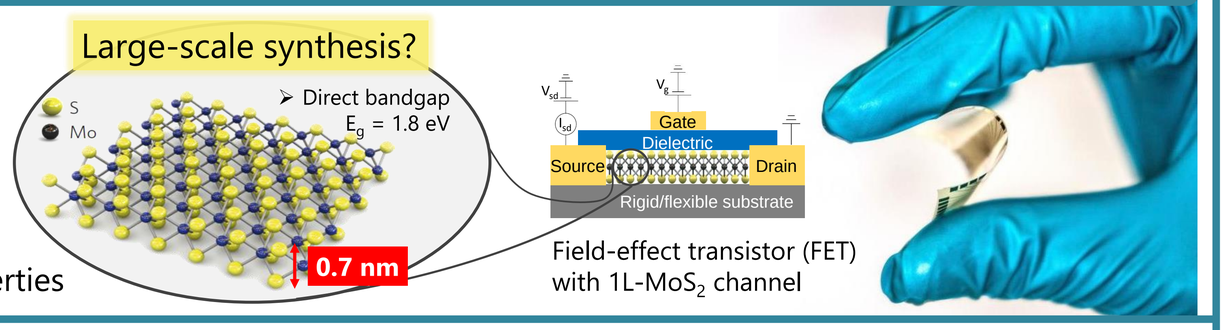
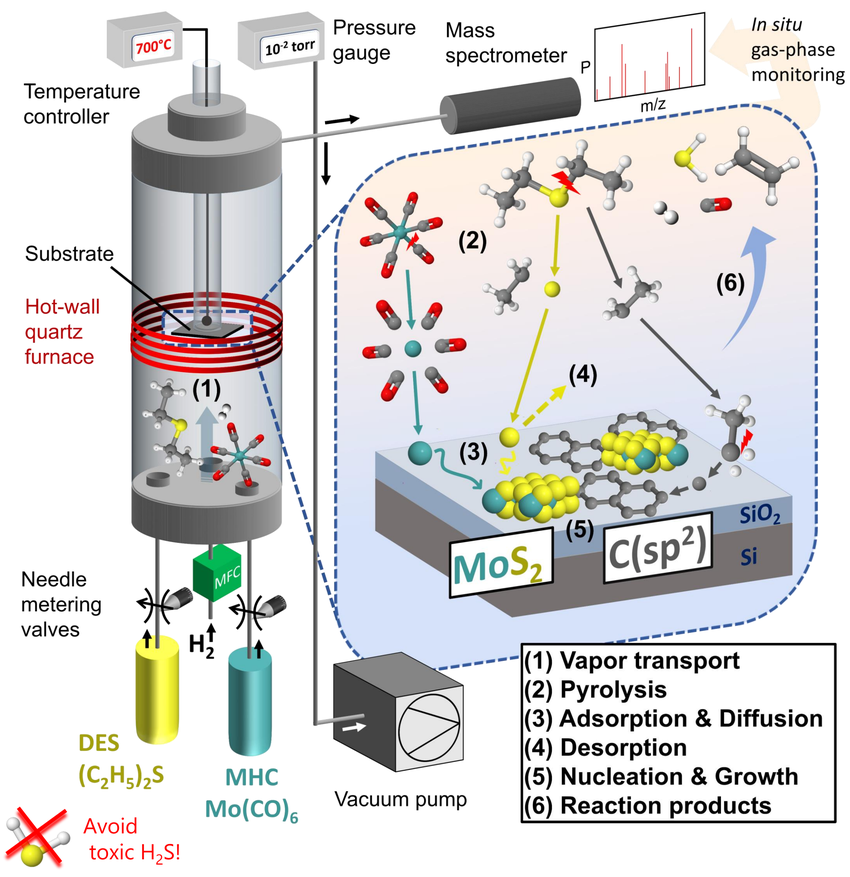
Motivation

- MoS_2 is an atomically-thin semiconductor suitable for (opto)electronic applications [1]
- Device commercialization requires controllable and scalable synthesis
  - ➢ Method: Metal-organic vapor deposition (MOCVD) [2]
- Use of low-cost, low-toxicity organic sulfur precursor preferred
  - ➢ Concern: carbon (C) incorporation affecting film growth and properties [3][4][5]

Goal: Understand mechanism behind C contamination and effect on film growth and properties

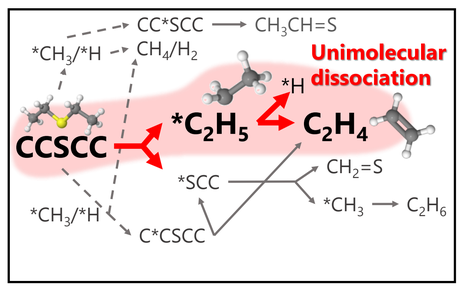


MoS_2 growth by MOCVD



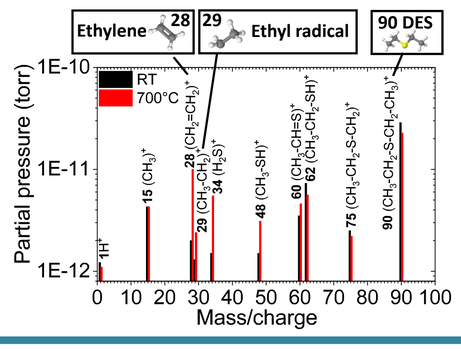
In situ gas-phase monitoring

DES pyrolysis pathway

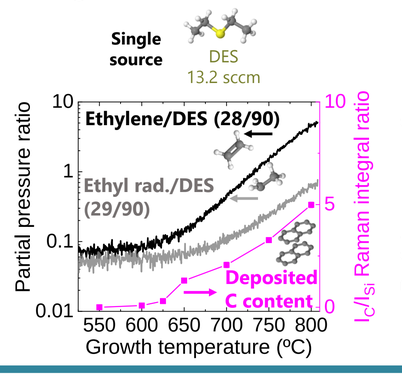


Zheng et al. (2009) [6]

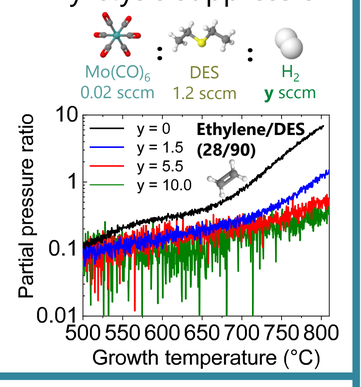
DES fragmentation pattern



Origin of C contamination

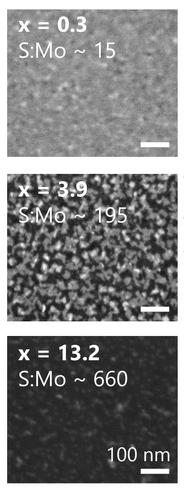


Pyrolysis suppression

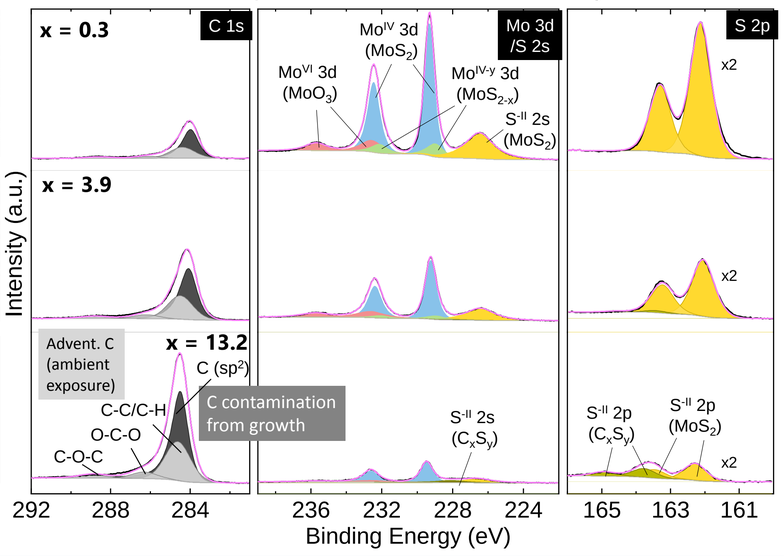


Effect of Mo:S precursor ratio on film properties

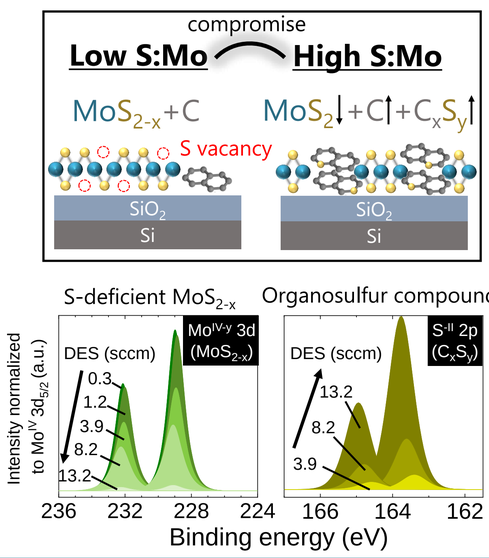
Morphology



Film composition and stoichiometry

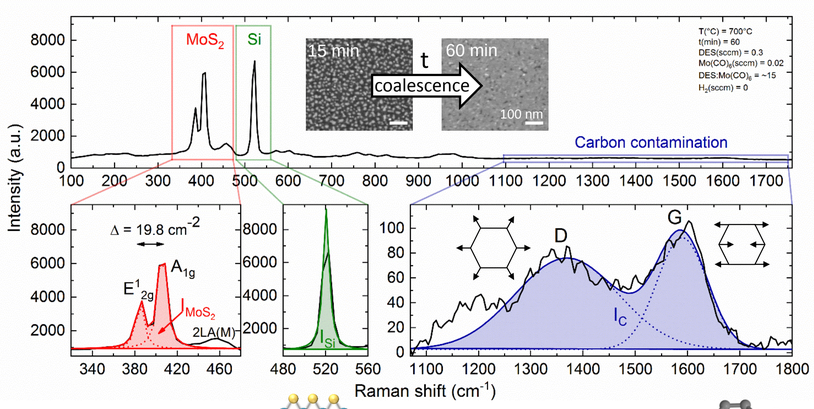


Gas mixture:
$Mo(CO)_6$ 0.02 sccm
+
DES **x** sccm



Semi-quantitative Raman spectroscopy

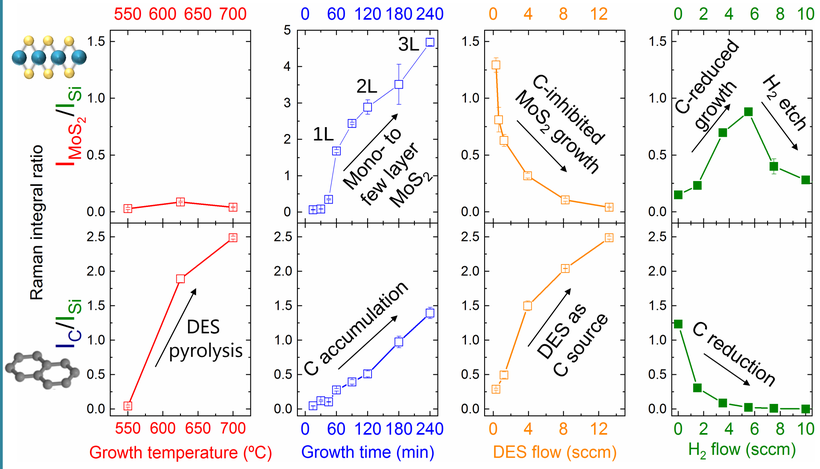
Carbon contamination in 1L-MoS_2



I_{MoS2}/I_{Si} ratio (MoS_2 content indicator)

I_C/I_{Si} ratio (Carbon content indicator)

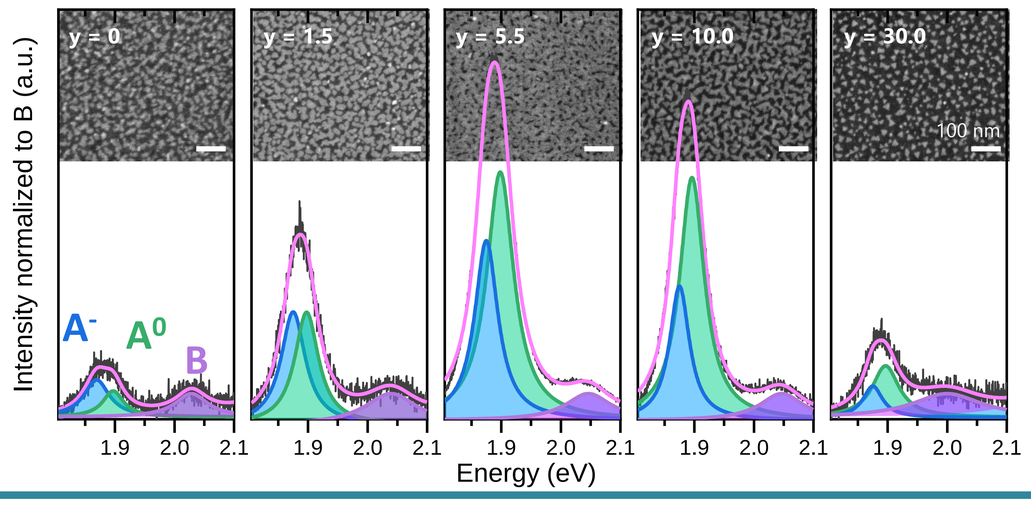
Growth parameter study



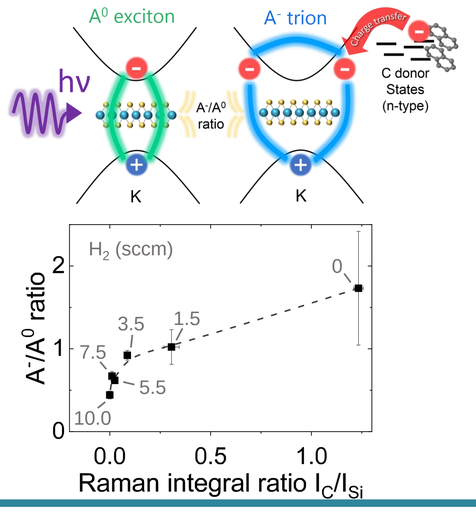
H_2-controlled carbon impurities & charge transfer doping

H_2 effect on morphology and photoluminescence

Gas mixture:
$Mo(CO)_6$ 0.02 sccm
+
DES 1.2 sccm
+
H_2 **y** sccm



Band diagram model



Conclusions

- Graphitic (sp^2) carbon contamination due to DES pyrolysis products (e.g. ethyl radicals, ethylene)
- C contamination at increased T above DES pyrolysis onset (~600ºC) and increased DES:$Mo(CO)_6$ ratios
- C contamination hinders lateral MoS_2 grain growth resulting in interrupted MoS_2 film morphology
- Use of organic S precursor compromises high Mo:S ratios required for stoichiometric MoS_2 growth
- Reductive H_2 suppresses DES pyrolysis and reduces C contamination even above 700°C
- Control over C impurity level enables tuneable charge transfer n-doping of MoS_2

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