Selective self-assembly of 2,3-diaminophenazine (DAP) molecules on $MoSe_2$ mirror twin boundaries

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Introduction & Motivation

- Two-dimensional transition metal dichalcogenides (TMDs) are fundamentally and technologically intriguing due to their versatile electronic, chemical and optical properties.
- Defects are inevitable in as-grown materials and strongly influence its properties.
- Dense metallic line defects, identified as mirror twin boundaries (MTBs) or inversion domain boundaries (IDBs), have been reported as an a striking property in MBE-grown $MoSe_2$ surface.
- The charge density wave (CDW) transition and spin charge separation have been revealed in metallic $MoSe_2$ MTBs by STM and ARPES measurements.
- However, the chemical properties and its influence on molecules of MTBs remain unexplored.

Results & Discussion

1 Structural and electronic properties of MBE-grown $MoSe_2$ on HOPG.

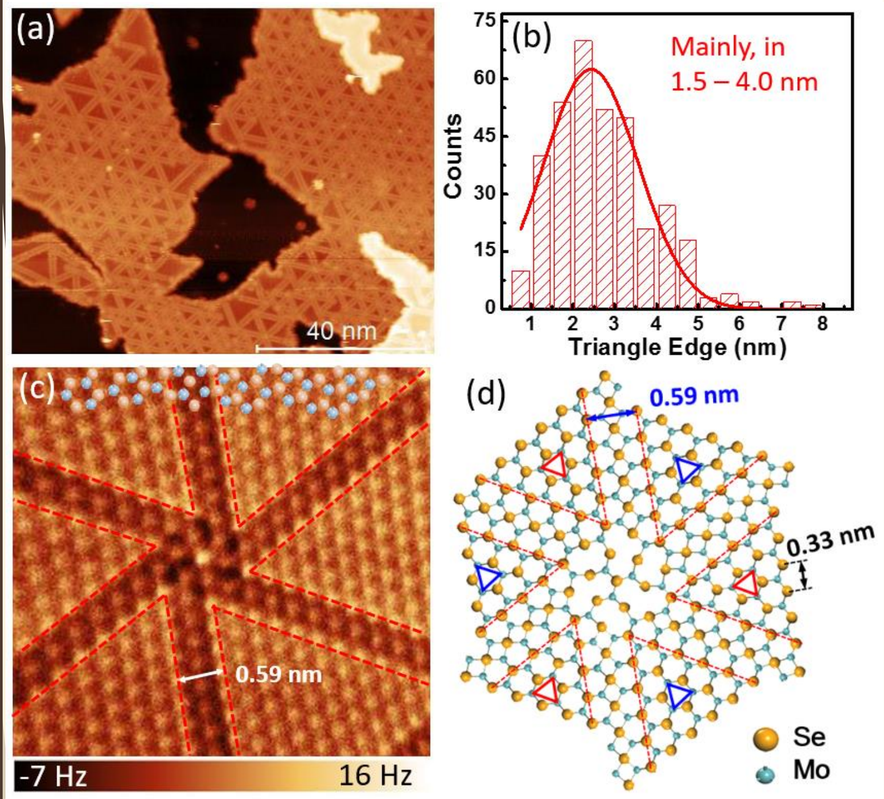


Fig 1. Triangle $MoSe_2$ domain and typical wagon-wheel patterns formed by MTBs.

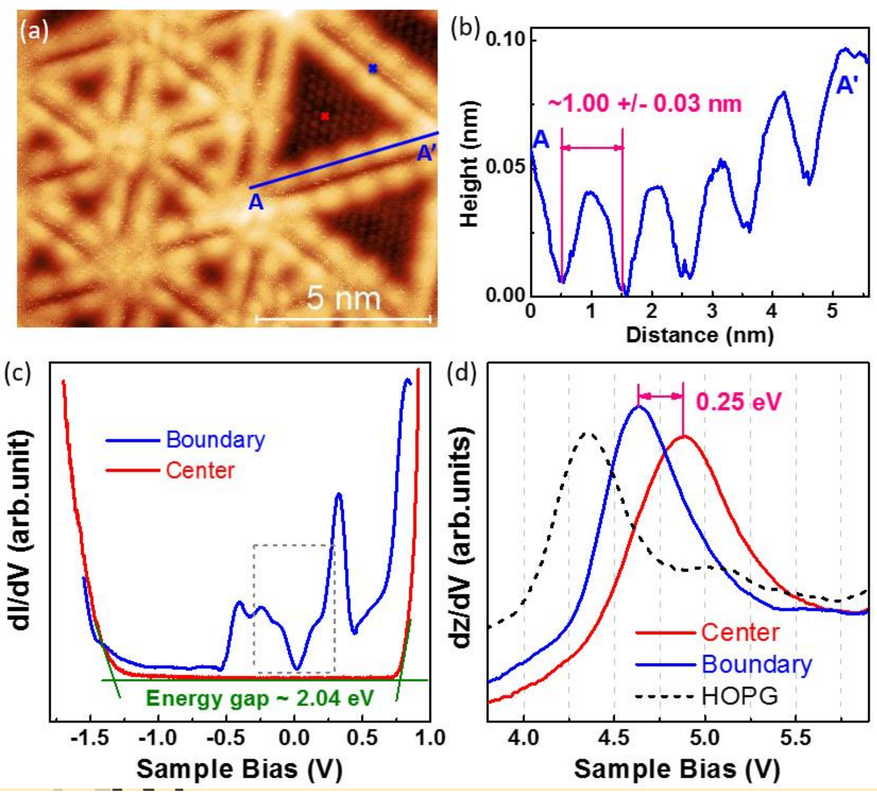


Fig 2. The metallic MTBs with lower work function (WK) compared with the semiconducting triangle MoSe2 domains.

2 DAP nano-porous network on wagon-wheel patterns of $MoSe_2$

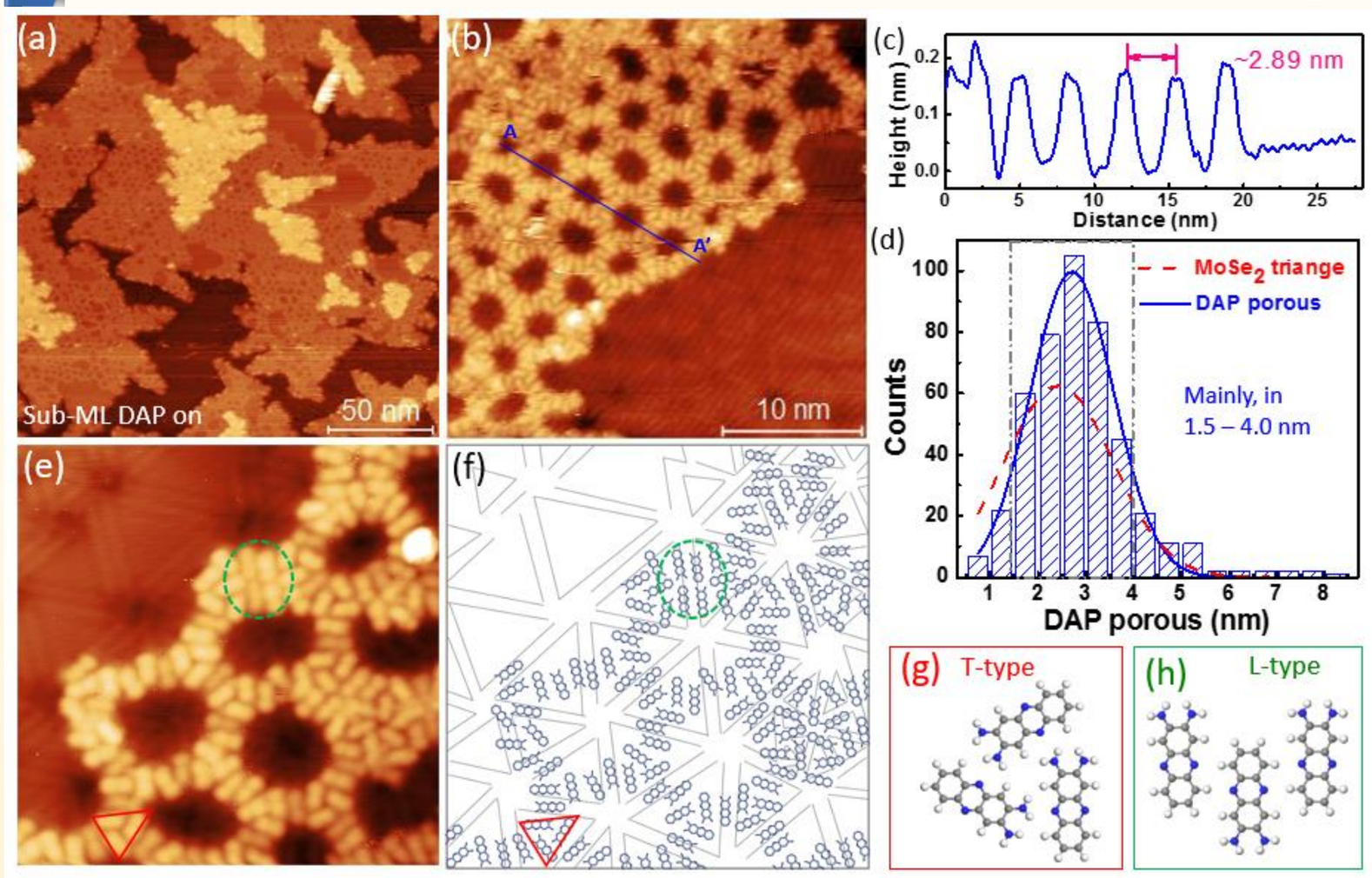
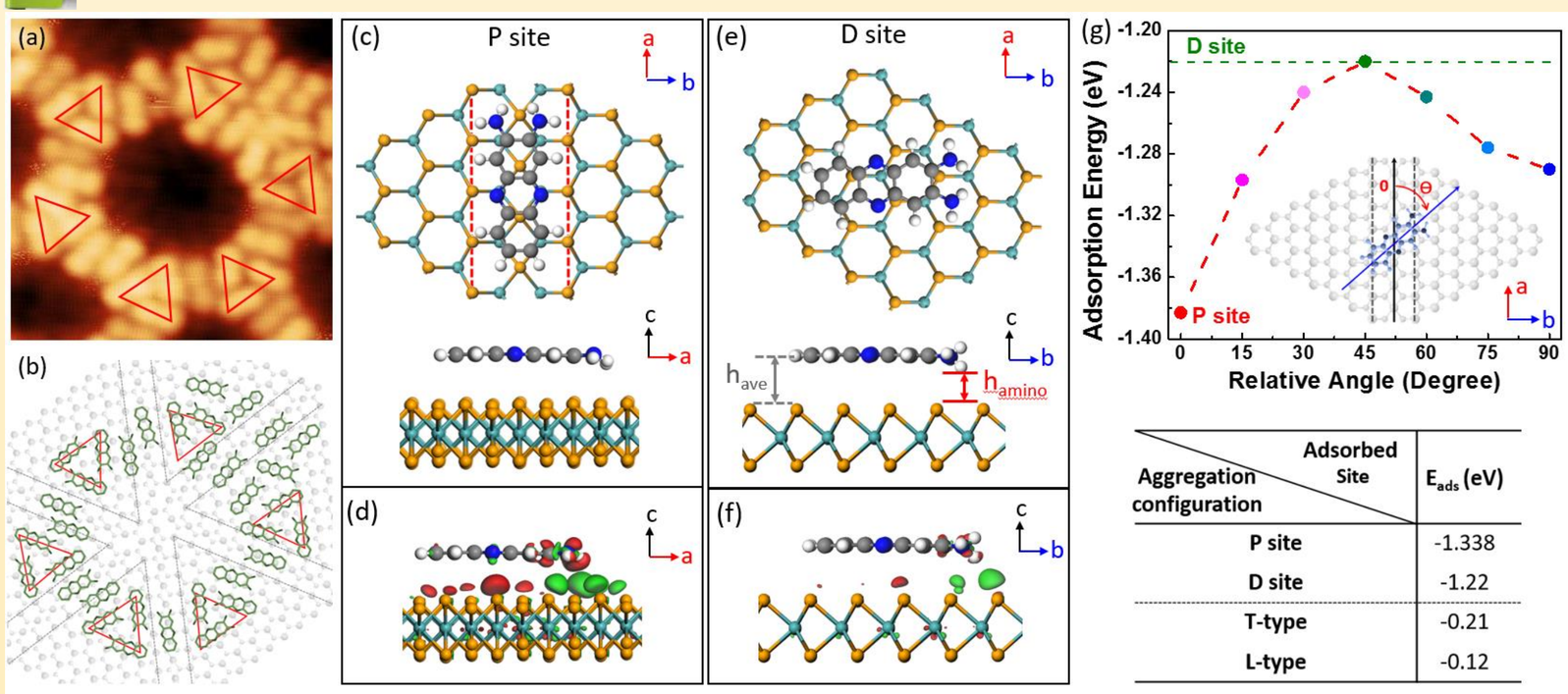


Fig 3. DAP pores with T-type aggregated configurations on triangle domain and L-type aggregated configurations on MTBs.

3 Formation mechanism of DAP pores and the influence of MTBs



Aggregation configuration \ Adsorbed Site	E_{ads} (eV)
P site	-1.338
D site	-1.22
T-type	-0.21
L-type	-0.12

Fig 4. The chemically activity of MTBs and amino-group of DAP play a critical role in forming the nanopores.

Summary

- The distinct structure of MTBs and wagon-wheel patterns of $MoSe_2$ were demonstrated by STM and nc-AFM images with high-resolution. MTBs was metallic and have lower WF.
- Sub-ML DAP molecules formed hexangular porous network on wagon-wheel patterns with L-type on MTBs as edge and T-type configuration on defect-free $MoSe_2$ as corner.
- The site-specific molecular self-assembly is attributed to the active MTBs couple with amino groups in the DAP molecules. Our results demonstrate the site-dependent electronic and chemical properties of $MoSe_2$ monolayers.