# Two Dimensional Decoupling Layers for Molecular Spectroscopy: TCNQ on $MoS_2$ Probed by LT-STM

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Organic molecules such as tetracyanoquinodimethane (TCNQ) are widely used as strong electron acceptors and serve as a model system for charge-transfer studies due to their high electron affinity and well-defined molecular orbitals. Upon adsorption on metallic substrates, the cyano groups strongly interact with surface d-orbitals, promoting the transfer of one electron into a low-lying molecular orbital and stabilizing TCNQ as a radical anion. This charge-transfer process, together with the resulting unpaired electron, underpins many of the electronic and magnetic functionalities that have made TCNQ central to the development of organic conductors and donor-acceptor materials [1].

Low-temperature scanning tunnelling microscopy (LT-STM) provides atomic-scale sensitivity to molecular adsorption geometries and enables visualization of molecular assemblies on different substrates. To study molecular phenomena in greater detail, ultrathin semiconducting layers can be introduced to reduce hybridization between molecules and metallic substrates. Among these materials, monolayer molybdenum disulfide ($MoS_2$) has emerged as a highly effective two-dimensional decoupling layer. $MoS_2$ consists of a single Mo layer in trigonal-prismatic coordination positioned between two sulfur layers and is held together by van der Waals forces. Its weak substrate interaction creates an intermediate coupling regime that preserves more of the intrinsic molecular electronic structure while still allowing high-resolution scanning probe access [2].

In this work, experiments were carried out using a LT-STM (CreaTec Fischer & Co. GmbH) under ultra-high vacuum conditions at 5 K. TCNQ molecules were evaporated onto $MoS_2$ monolayers grown on Au(111). Molybdenum was deposited onto the clean Au(111) surface, prepared by repetitive cycles of $Ne^+$ sputtering and annealing in a $H_2S$ atmosphere of $10^{-5}$ mbar by electron-beam evaporation from a high-purity rod. The sample was annealed at 530 °C subsequently. The STM images reveal TCNQ networks formed both on $MoS_2$ patches and on bare Au(111), allowing direct comparison between weakly and strongly coupled adsorption environments. Scanning tunnelling spectroscopy (STS) was then used to probe the electronic structure of TCNQ molecules in these distinct environments.

The STS results for TCNQ adsorbed on $MoS_2$ show that the lowest unoccupied molecular orbital (LUMO) is significantly narrower than on the bare substrate. The spectra also display clear vibronic progressions within the unoccupied molecular resonances [3].

These results demonstrate that monolayer $MoS_2$ acts as an effective decoupling layer for molecular spectroscopy of charge-transfer acceptor molecules. The vibronic features observed in the STS spectra indicate that $MoS_2$ partially isolates the molecular orbitals from the metallic substrate, allowing features that are typically suppressed under strong hybridization to be resolved.

## REFERENCES

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