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LUCES

Supramolecular LUminescent Chemosensors for Environmental Security

Central-metal-controlled charge-transfer pathways in CuPc-, FePc- and MgPc-functionalized WS_2 for NO_2 sensing interfaces

Two-week visit at the University of Barcelona to develop an electronic and mechanistic interpretation of MPc-functionalized WS_2 chemiresistive sensors.

Experimental characterization

A dataset for pristine WS_2 and CuPc-, FePc- and MgPc-functionalized WS_2 sensors was consolidated for comparative analysis. It included morphology, Raman and XRD, UV-vis, I–V curves, NO_2 response–recovery traces, humidity-effect and stability.

Electronic analysis

Together with Prof. Frank Güell Vilà's group, the experimental dataset was interpreted using electronic-structure analysis. Vacuum-referenced energy-level alignment between WS_2 and CuPc/FePc/MgPc was examined to understand central-metal-dependent interfacial charge transfer.

Mechanism & outputs

The CuPc–WS_2, FePc–WS_2 and MgPc–WS_2 comparison was organized into a charge-transfer mechanism map linking central-metal identity to interfacial carrier modulation and NO_2 sensing performance. The visit also defined follow-up analyses and the mechanistic framework for a joint manuscript.

This STSM combined experimental characterization with a mechanistic interpretation of MPc-functionalized WS_2 sensing interfaces. The visit studied the link between molecular functionalization, charge transfer and device performance, supporting LUCES objectives by connecting materials chemistry with device-level interpretation.

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