Supporting Information for

Unravelling Work Function Contributions and Their Engineering in 2 2H-MoS2 Single Crystal Discovered by Molecular Probe Interaction

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Figure S1 shows the C 1s, O 1s and N 1s core levels of as-received MoS₂ single crystal and after solvent-cleaning and blowing dry with nitrogen, proving that in both cases neither carbon, oxygen nor nitrogen were present on the pristine MoS₂ sample.

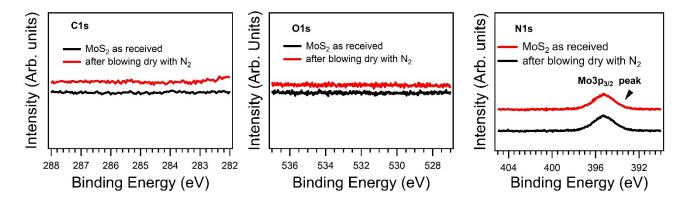


Figure S1. C 1s, O 1s and N 1s core levels of as-received MoS₂ single crystal and after solventcleaning and nitrogen blowing.

Figure S2 displays the C 1s and O 1s core levels of thiol-functionalized (thermally treated) MoS₂ sample, exhibiting components with the correct relative weight (i.e., intact molecule).

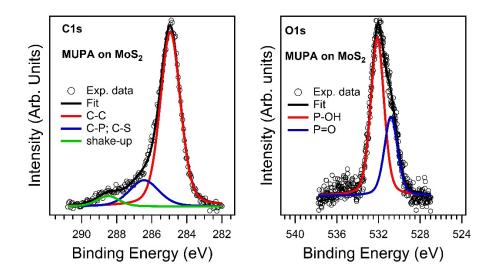


Figure S2. C 1s and O 1s core levels of thiol-functionalized (thermally treated) MoS₂ single crystal.