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Supporting Information

for

DFT calculations of the structure and stability of copper clusters on MoS_2

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Additional computational data

DOS Plots

Density of state plots for all Cu_n adsorption configurations are given below.



Figure S1: DOS plots of Cu_1 and Cu_2 adsorption structures. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of 5 for the ease of comparison.



Figure S2: DOS plots of Cu_3 adsorption structures. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of five for the ease of comparison.



Figure S3: DOS plots of Cu_4 adsorption structures. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of five for the ease of comparison.



Figure S4: DOS plots of Cu_1 and Cu_4 adsorption structures on defective MoS_2 . Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of five for the ease of comparison.

Charge Density Distribution after adsorption of Cu_n

The charge density difference after adsorption of the most favourable Cu_n is shown below.



Figure S5: Charge density difference after adsorption of the most favourable Cu_n on pristine (A–G) and defective (H, I) MoS₂.

Cu atom repelled from ML

An example of a Cu atom that is repelled from the MoS_2 ML is shown in Figure S6. This occurred during the relaxation of several Cu₄ structures on the MoS_2 monolayer with an S vacancy.



Figure S6: A Cu atom is repelled from the surface during the geometry relaxation.