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Supporting Information

for

DFT calculations of the structure and stability of copper clusters on MoS$_2$

Cara-Lena Nies and Michael Nolan

*Beilstein J. Nanotechnol.* 2020, 11, 391–406. doi:10.3762/bjnano.11.30

Additional computational data
DOS Plots

Density of state plots for all Cu$_n$ adsorption configurations are given below.
**Figure S1:** DOS plots of Cu₁ and Cu₂ 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\textsubscript{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.

![Charge density distribution](image)

**Figure S5:** Charge density difference after adsorption of the most favourable Cu$_n$ on pristine (A–G) and defective (H, I) MoS$_2$. 

S7
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 Cu$_4$ structures on the MoS$_2$ monolayer with an S vacancy.

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