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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.

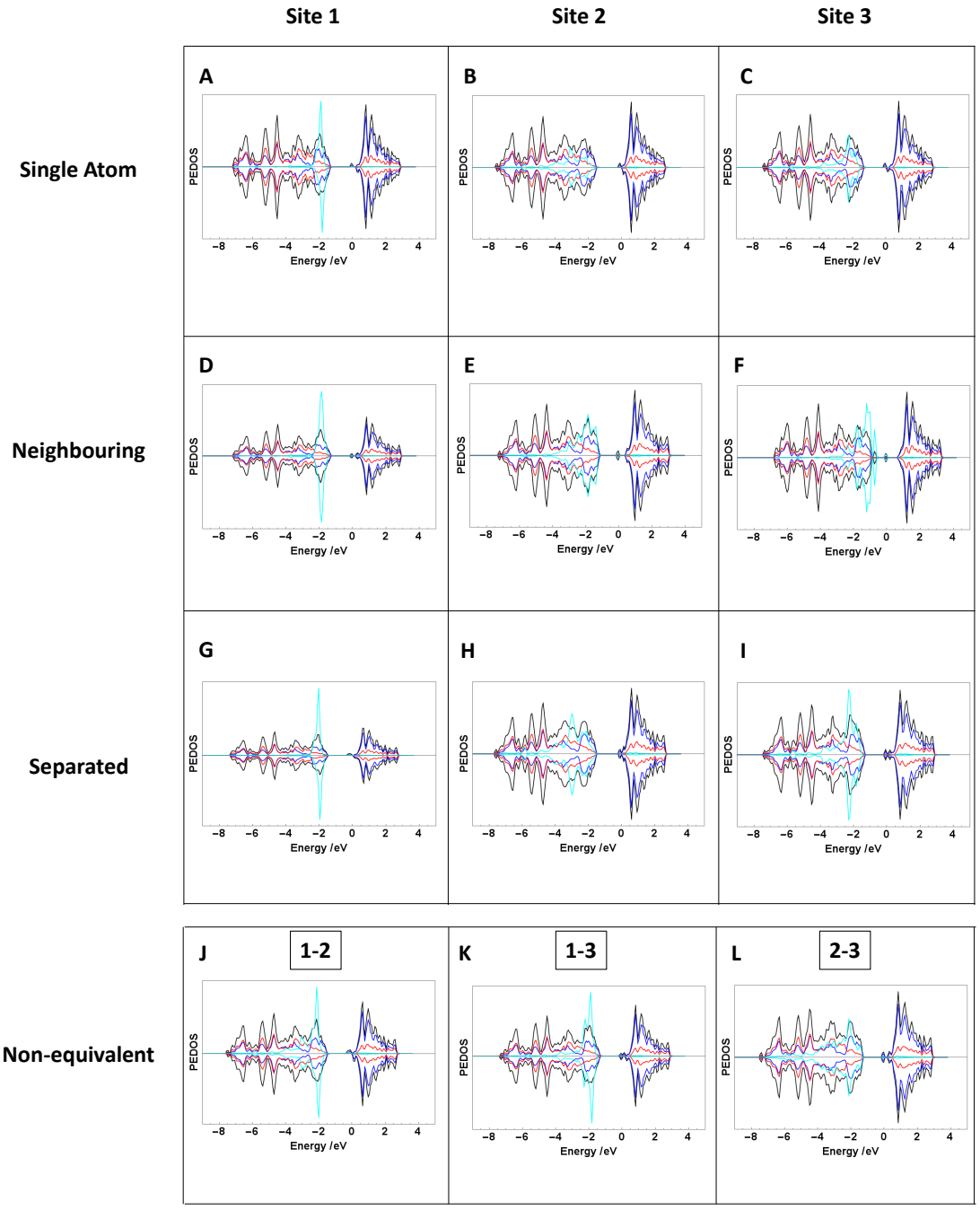


**Figure S1:** DOS plots of $Cu_1$ and $Cu_2$ adsorption structures. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of 5 for the ease of comparison.

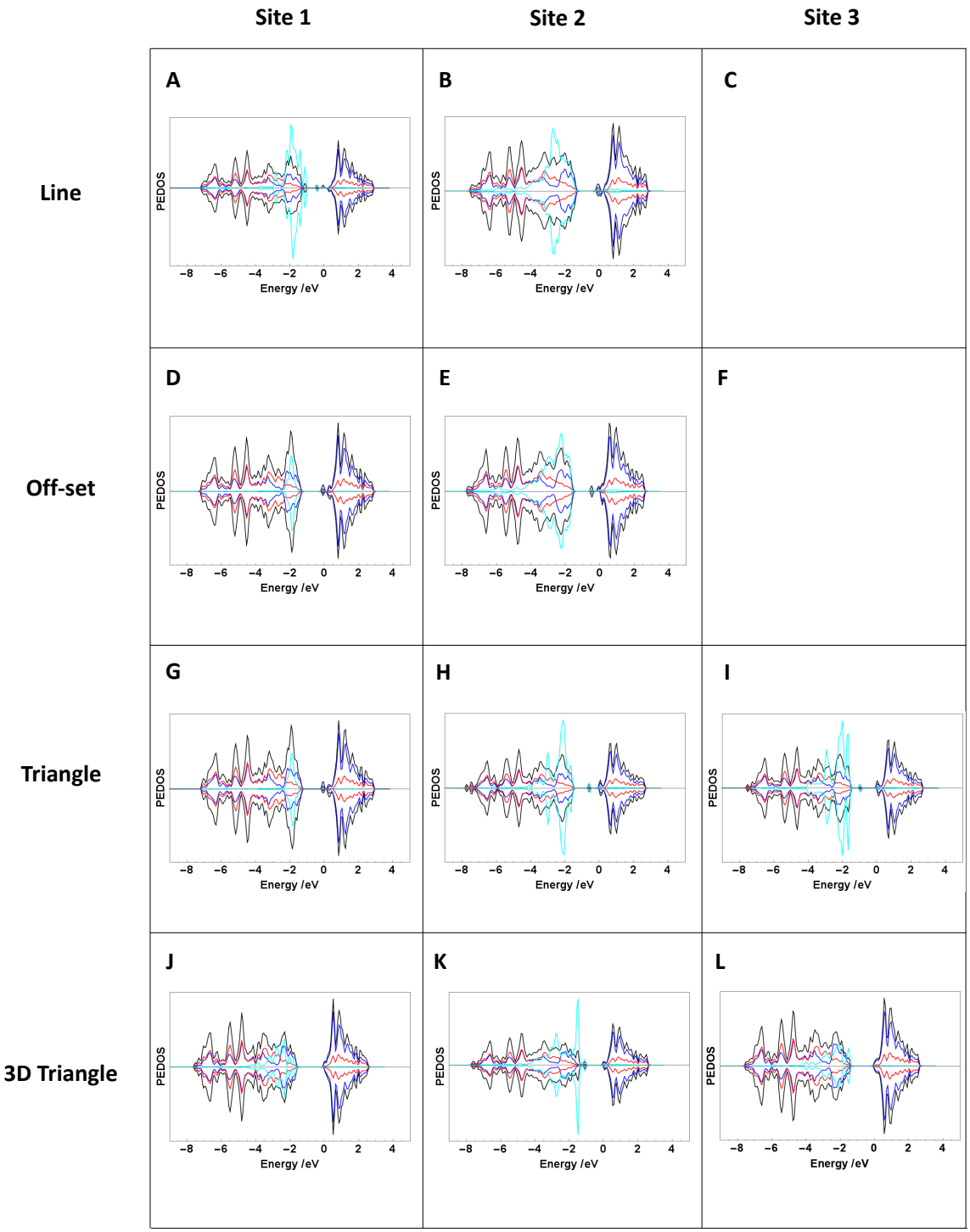


**Figure S2:** DOS plots of $Cu_3$ adsorption structures. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of five for the ease of comparison.

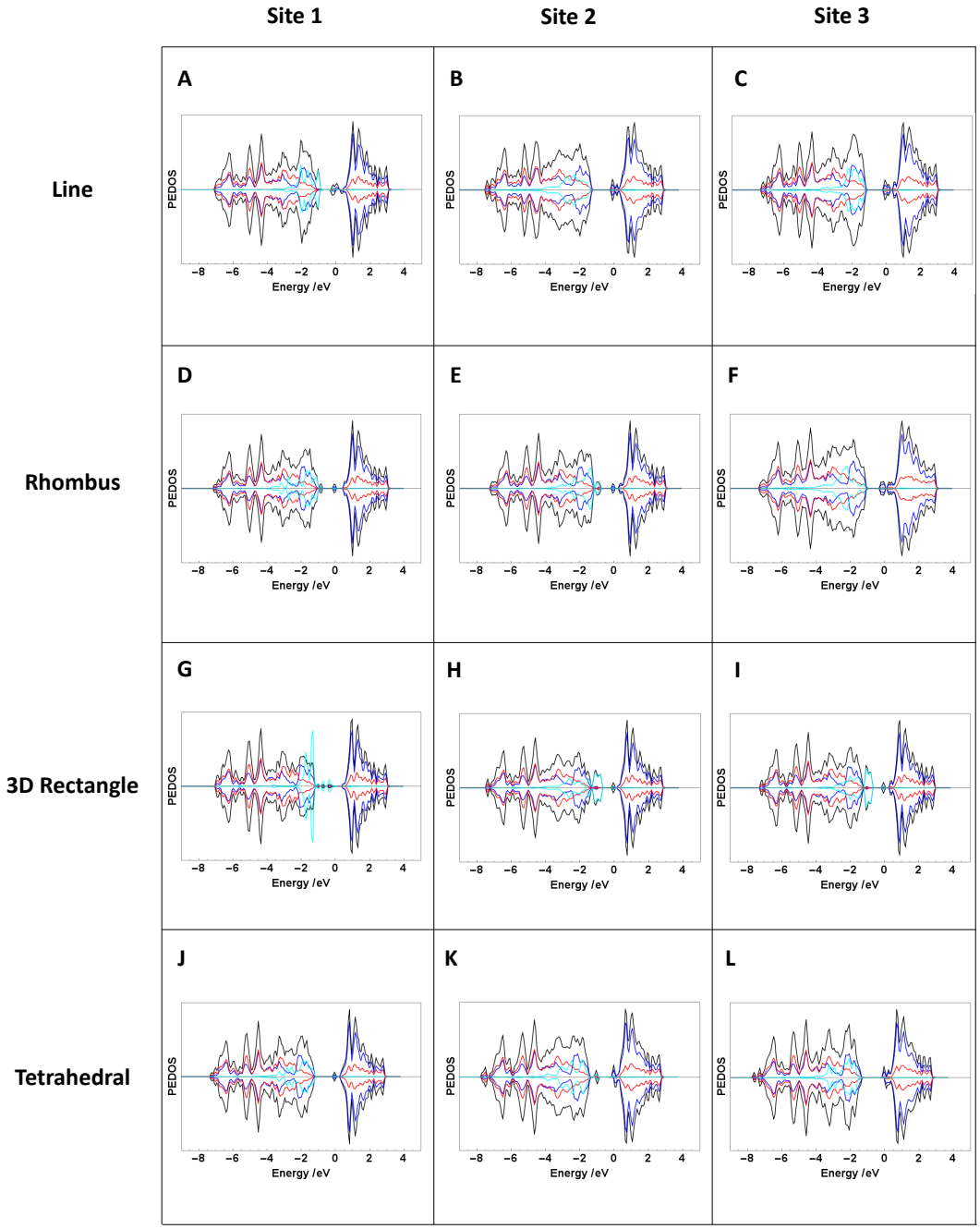


**Figure S3:** DOS plots of $Cu_4$ adsorption structures. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of five for the ease of comparison.

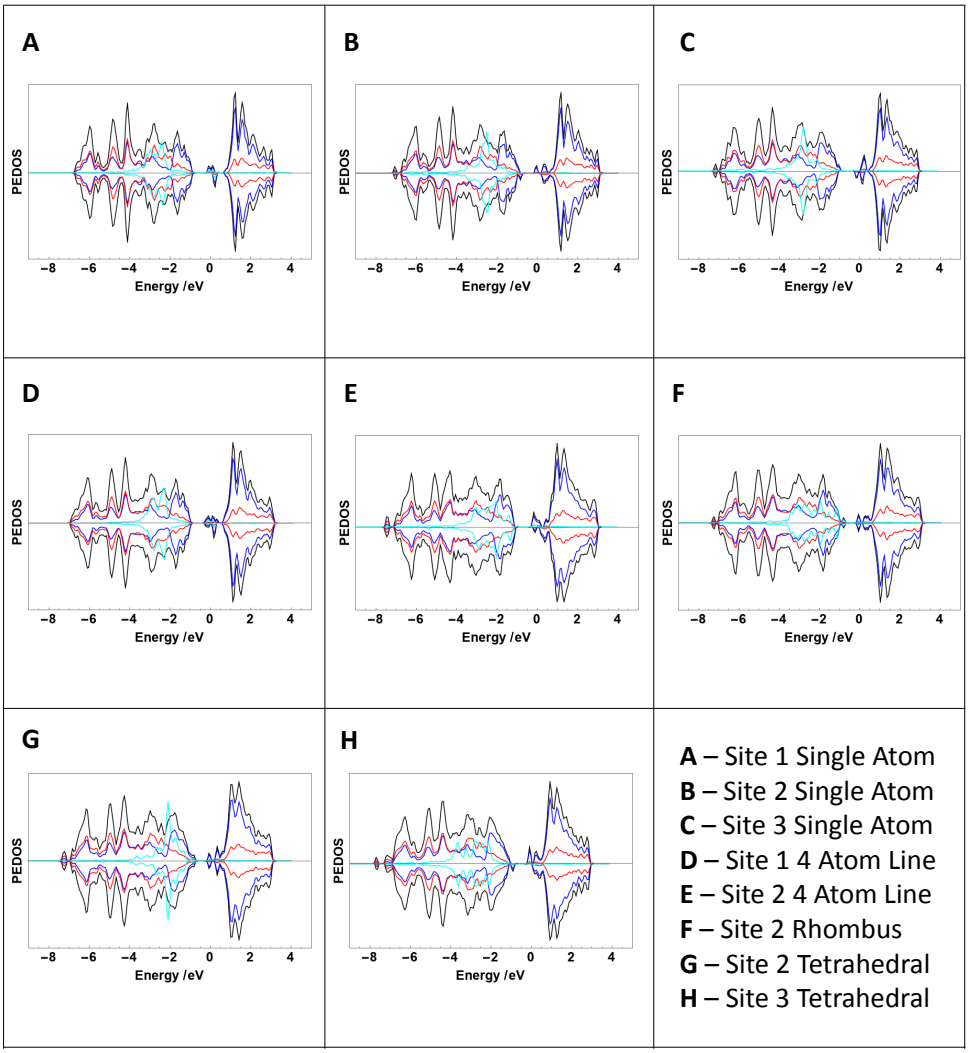


**Figure S4:** DOS plots of $Cu_1$ and $Cu_4$ adsorption structures on defective $MoS_2$. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of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

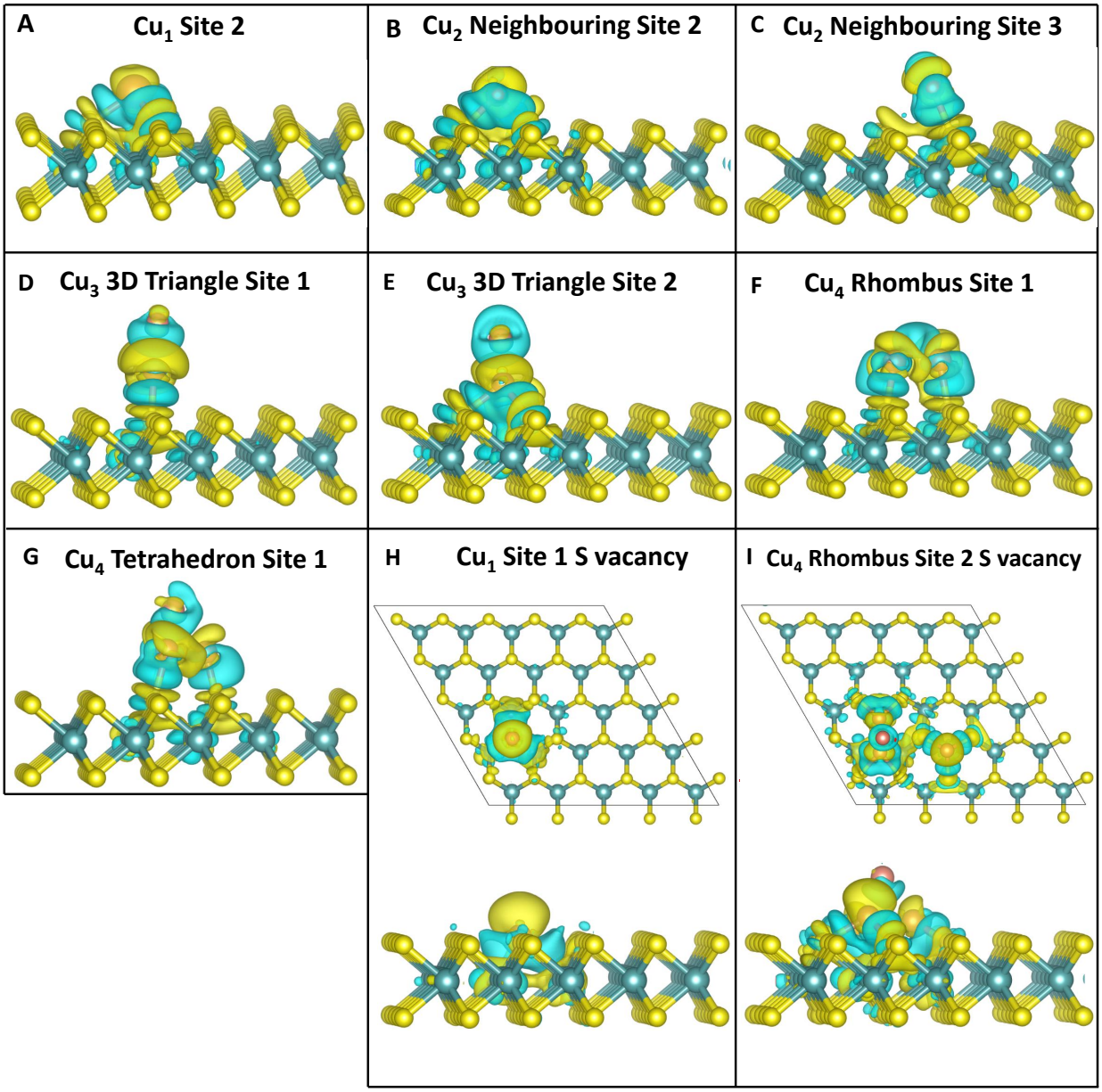


**Figure S5:** Charge density difference after adsorption of the most favourable $Cu_n$ on pristine (A–G) and defective (H, I) $MoS_2$.

## 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.

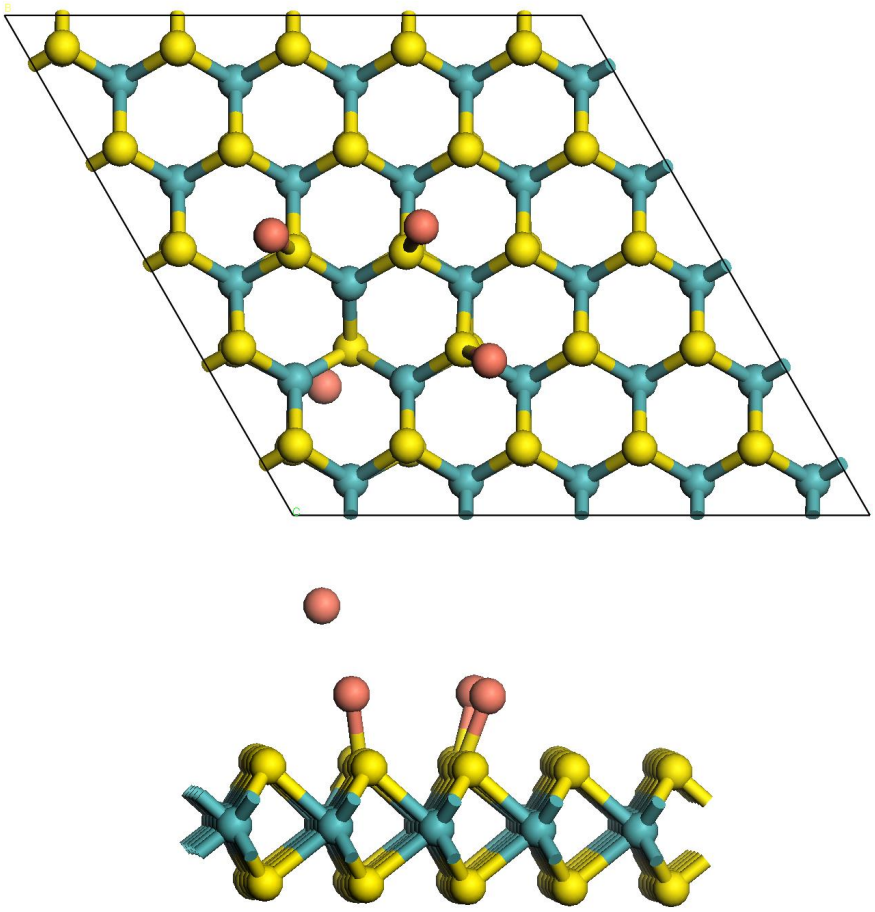

**Figure S6:** A Cu atom is repelled from the surface during the geometry relaxation.