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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

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Additional computational data

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DOS Plots

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

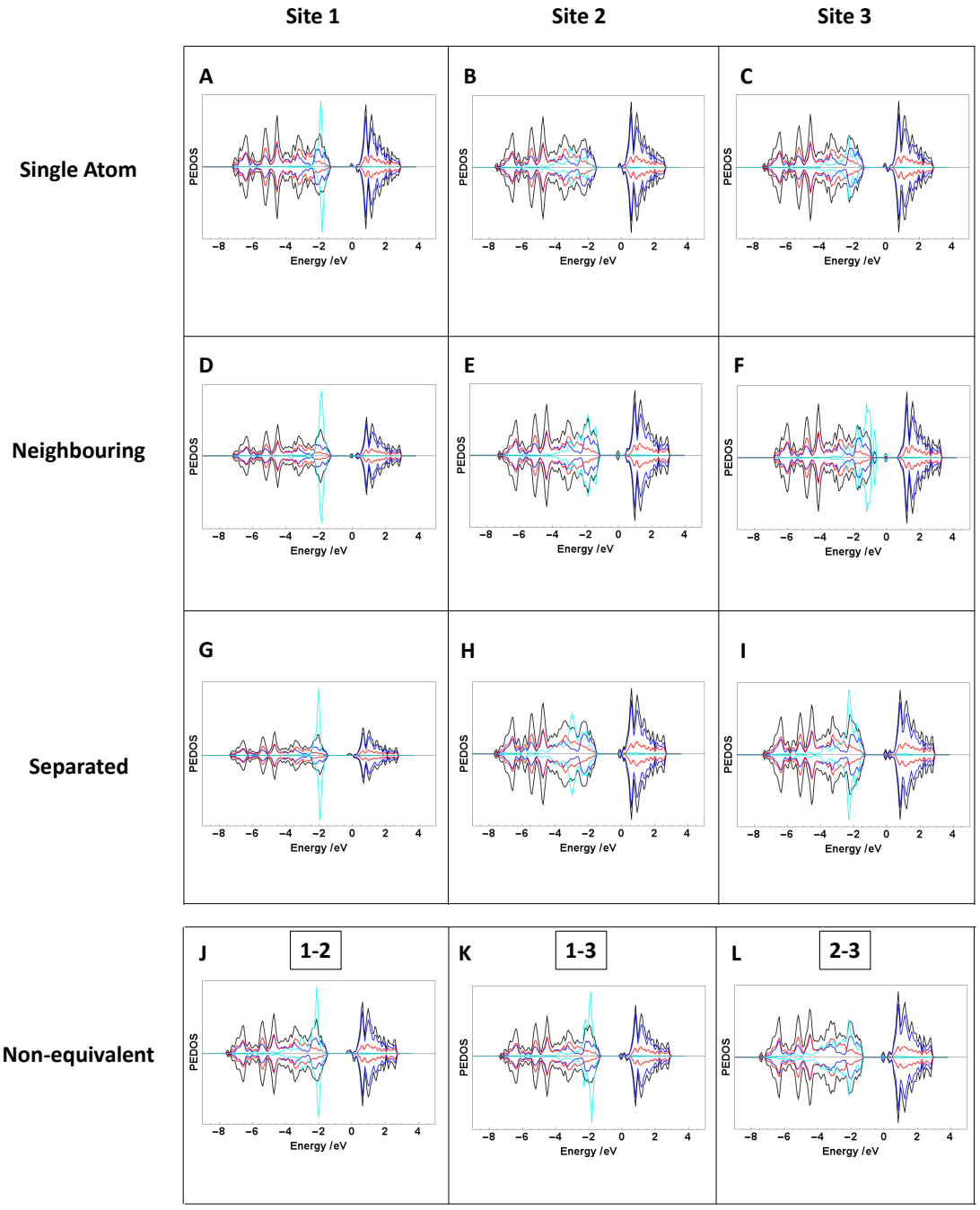


Figure S1: DOS plots of Cu_1 and Cu_2 adsorption structures. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of 5 for the ease of comparison.

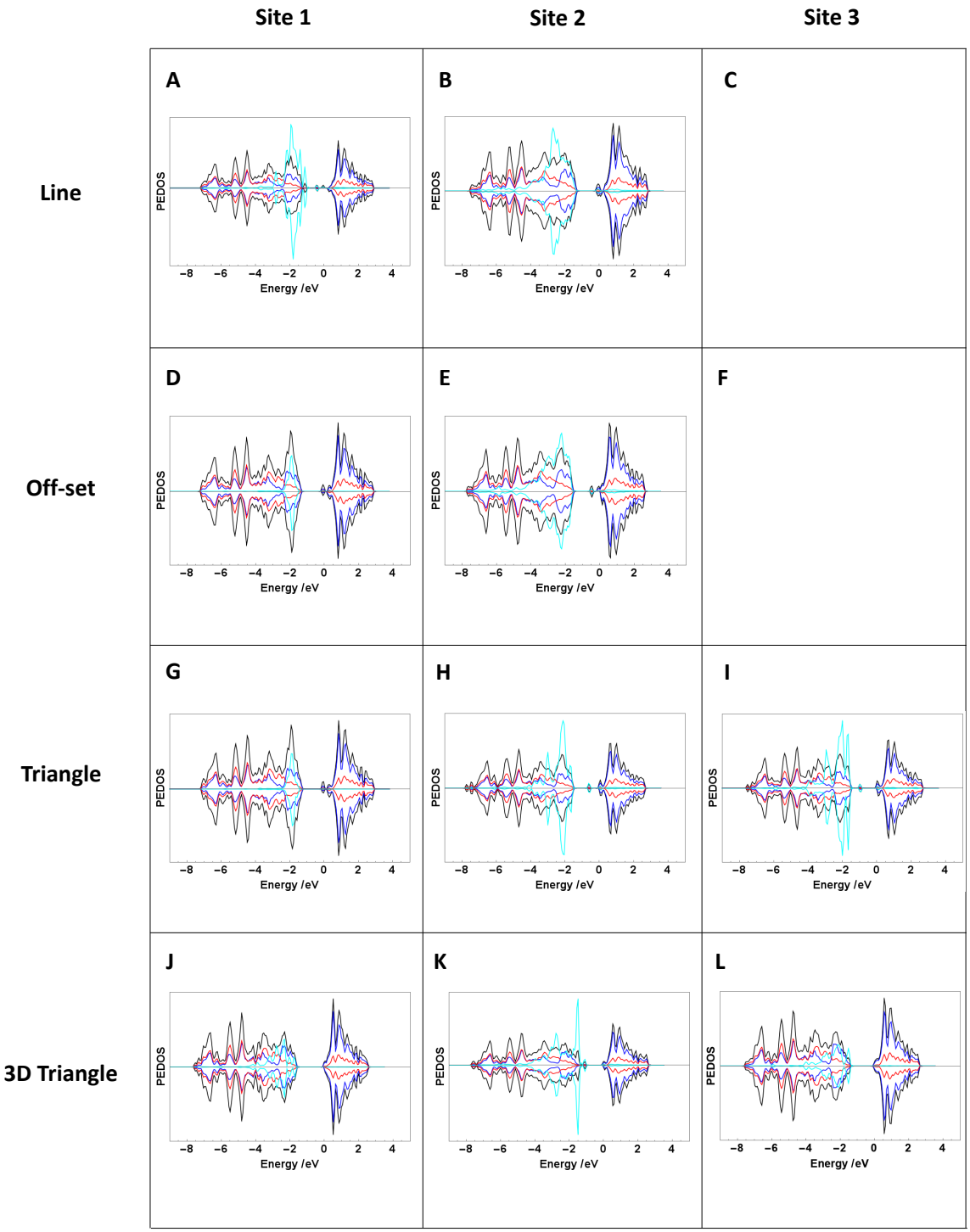


Figure S2: DOS plots of Cu_3 adsorption structures. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of five for the ease of comparison.

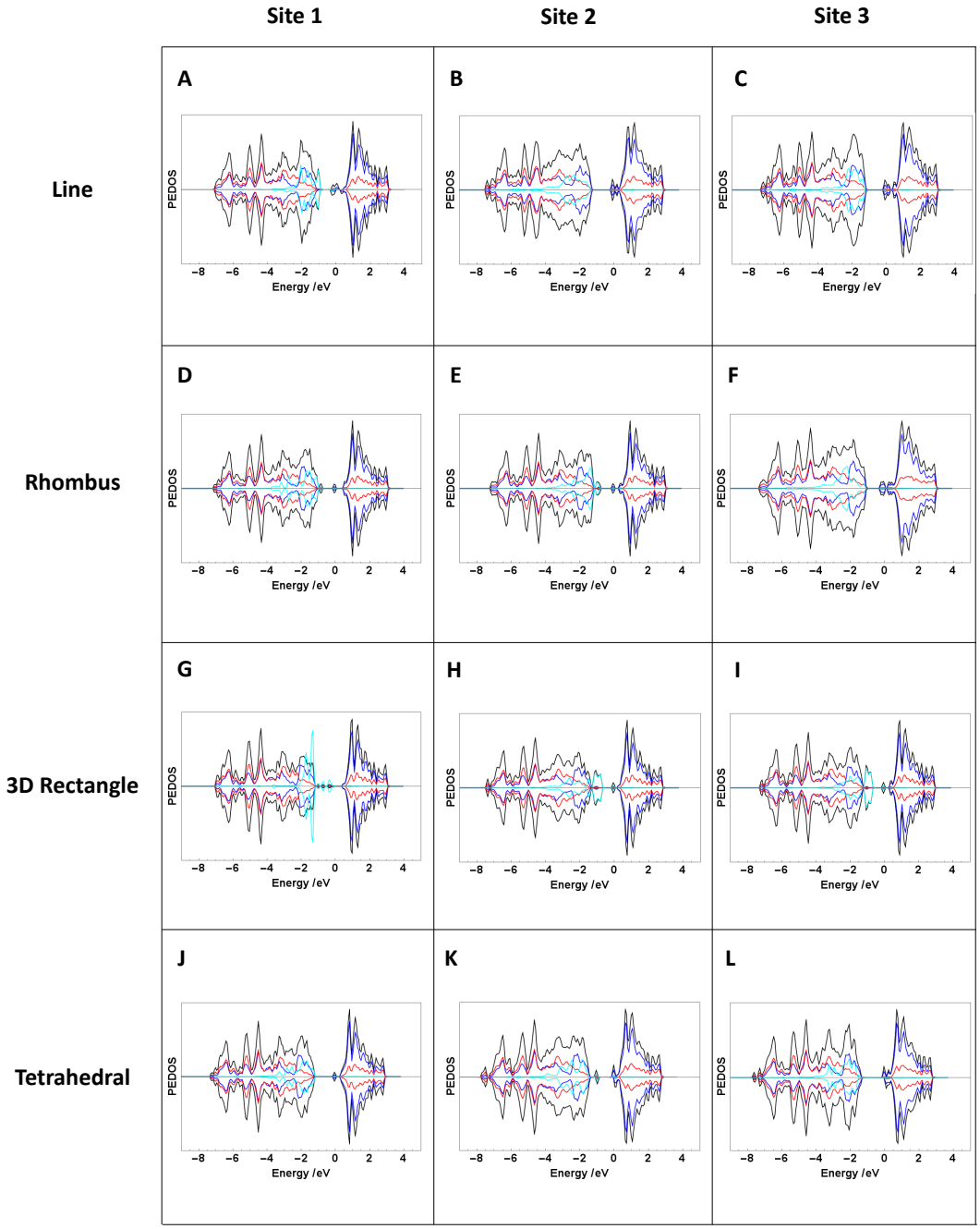


Figure S3: DOS plots of Cu_4 adsorption structures. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of five for the ease of comparison.

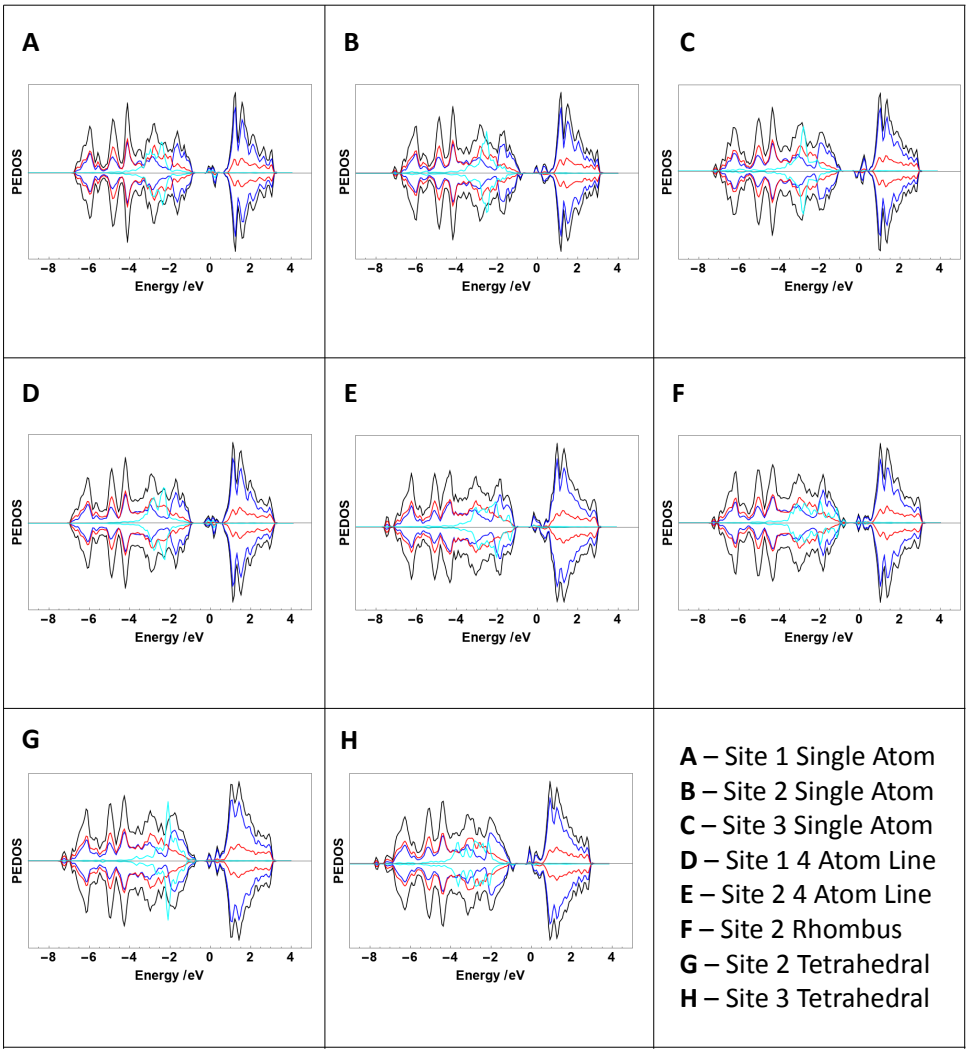


Figure S4: DOS plots of Cu_1 and Cu_4 adsorption structures on defective MoS_2. Black = total DOS, blue = DOS projected onto Mo d orbitals, red = DOS projected onto S p orbitals, cyan = DOS projected onto Cu d orbitals. The contribution of the Cu d orbitals has been increased by a factor of five for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

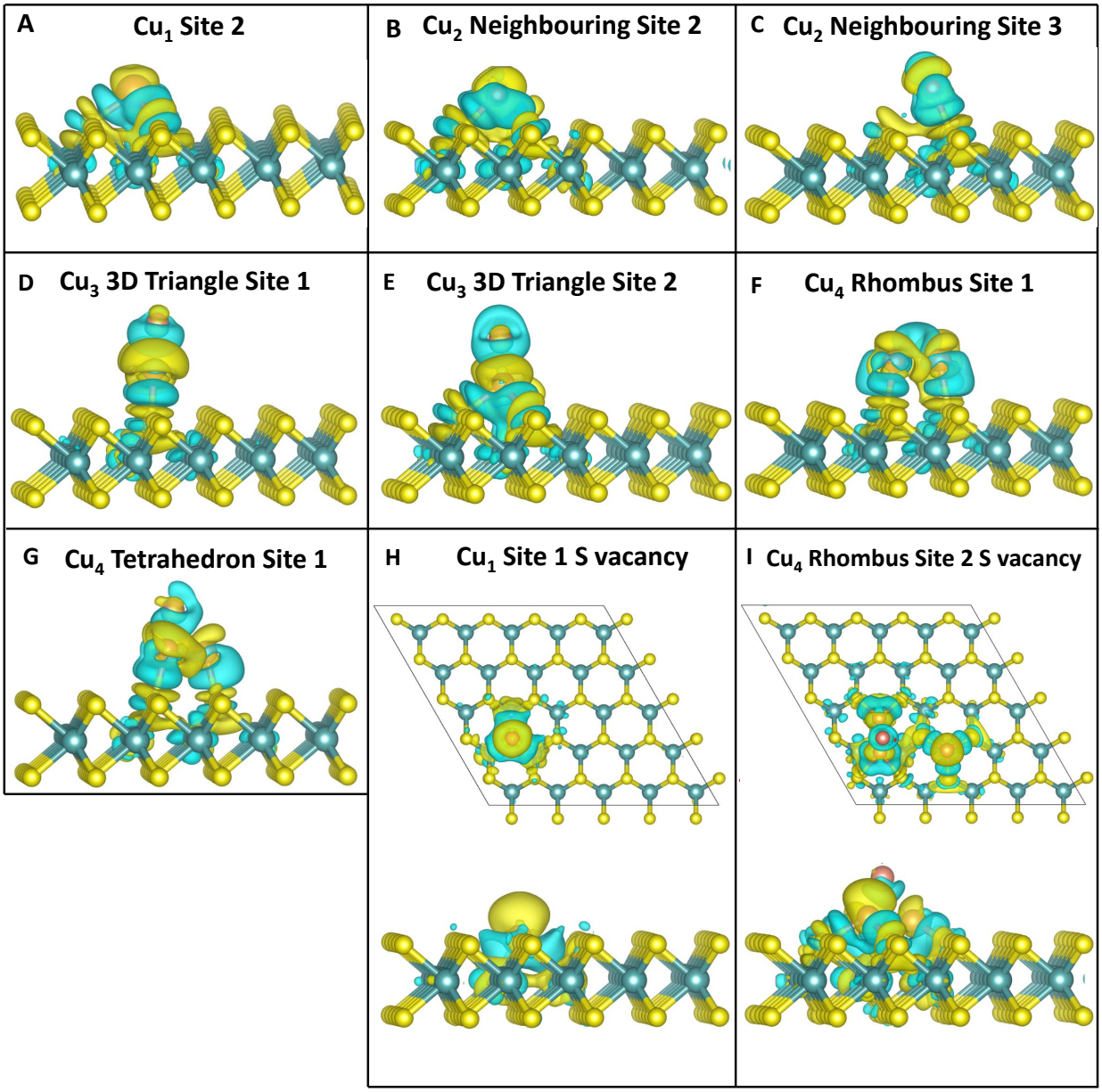


Figure S5: Charge density difference after adsorption of the most favourable Cu_n on pristine (A–G) and defective (H, I) MoS_2.

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.

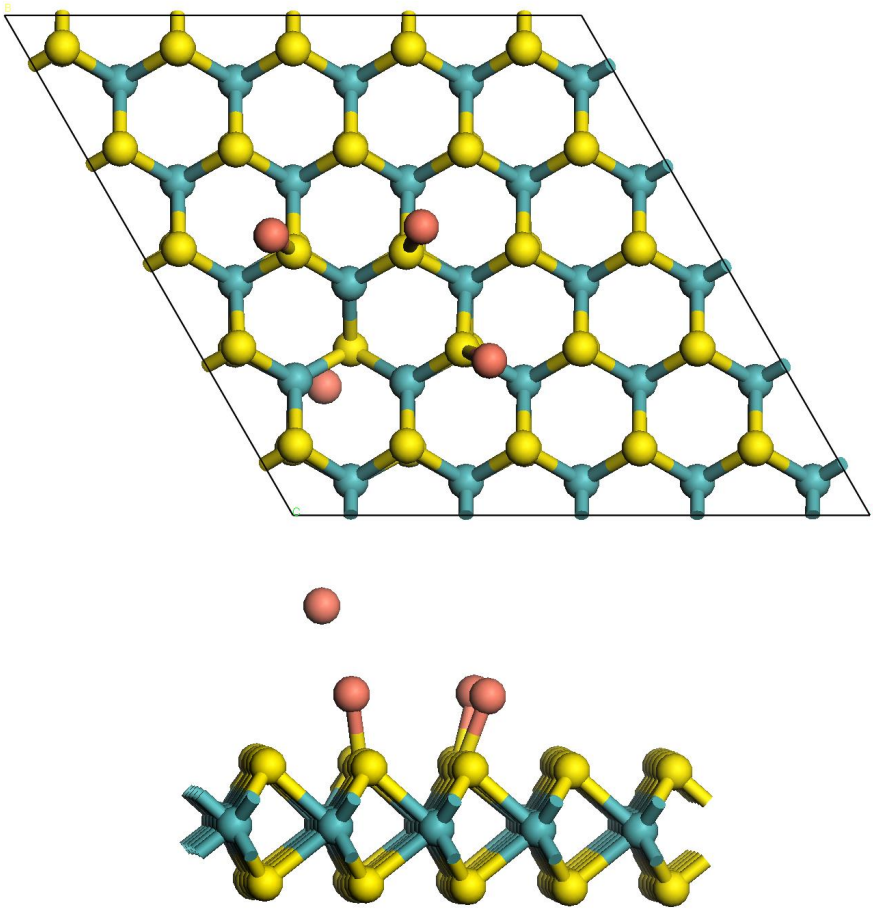


Figure S6: A Cu atom is repelled from the surface during the geometry relaxation.