Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information (ESI): Exploring Adsorption Behavior of Sulfur and Nitrogen Compounds on Transition Metal-Doped Cu (100) Surfaces: Insights from DFT and MD Simulations

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Additional computational analysis

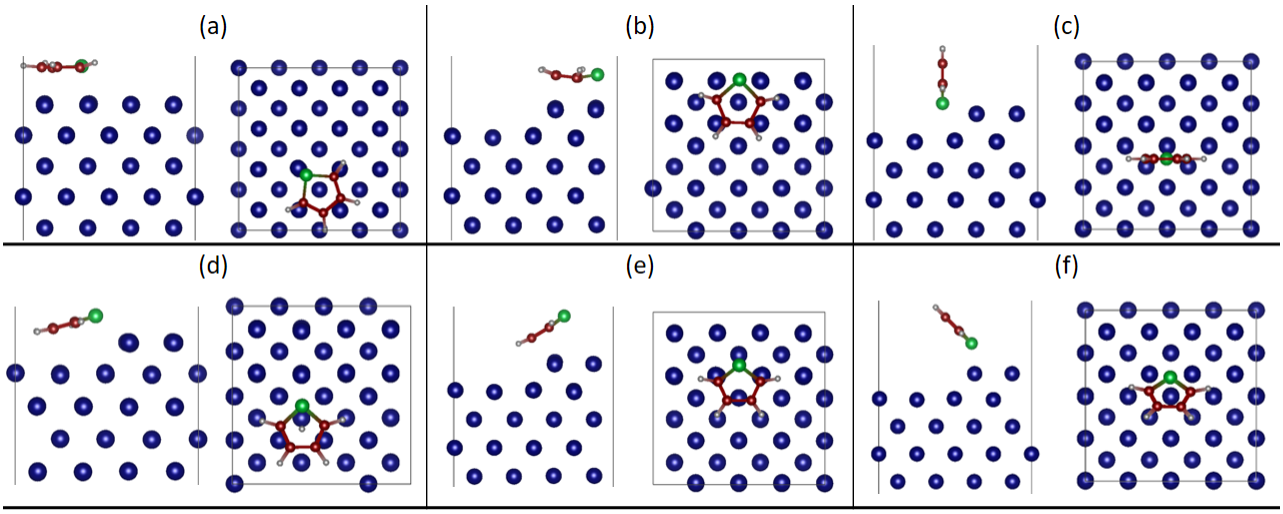

Figure S1: Top and side views of configurations for adsorption of thiophene on perfect (a) and defective Cu (100) surface: (b) f-upper terrace, (c) v-lower terrace, (d) f-lower terrace, (e) f-step, and (f) inclined configuration.
Blue, green, grey, and dark red balls represent copper, sulfur, hydrogen, and carbon atoms, respectively.

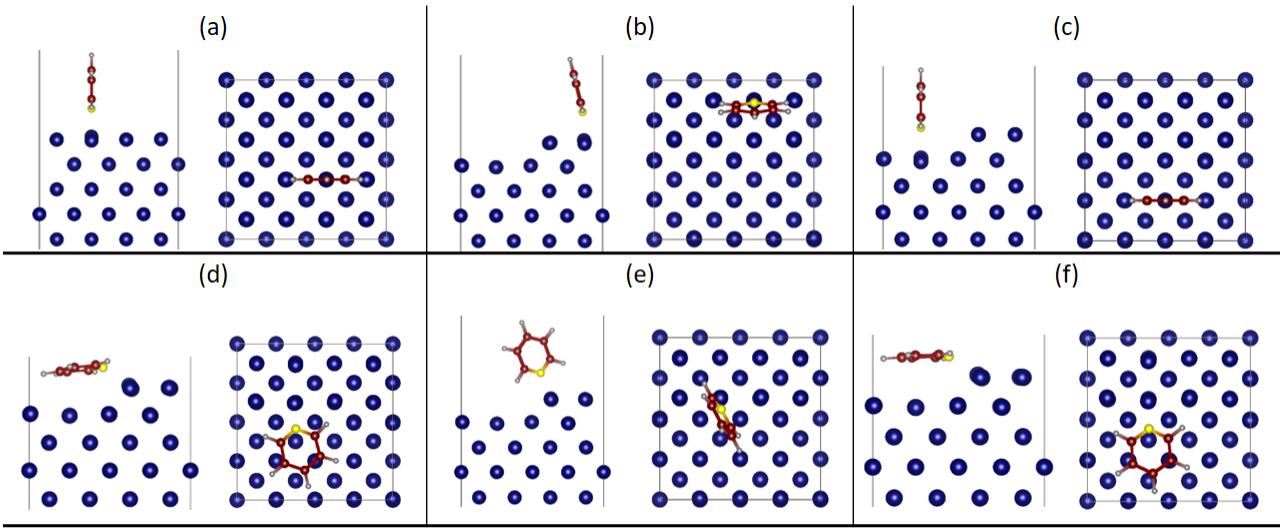

Figure S2: Top and side views of configurations for adsorption of pyridine on perfect (a) and stepped Cu (100) surface: (b) v-upper terrace, (c) v-lower terrace, (d) f-lower terrace, (e) v-step, and (f) inclined configuration.
Blue, yellow, grey, and dark red balls represent copper, nitrogen, hydrogen, and carbon atoms, respectively.

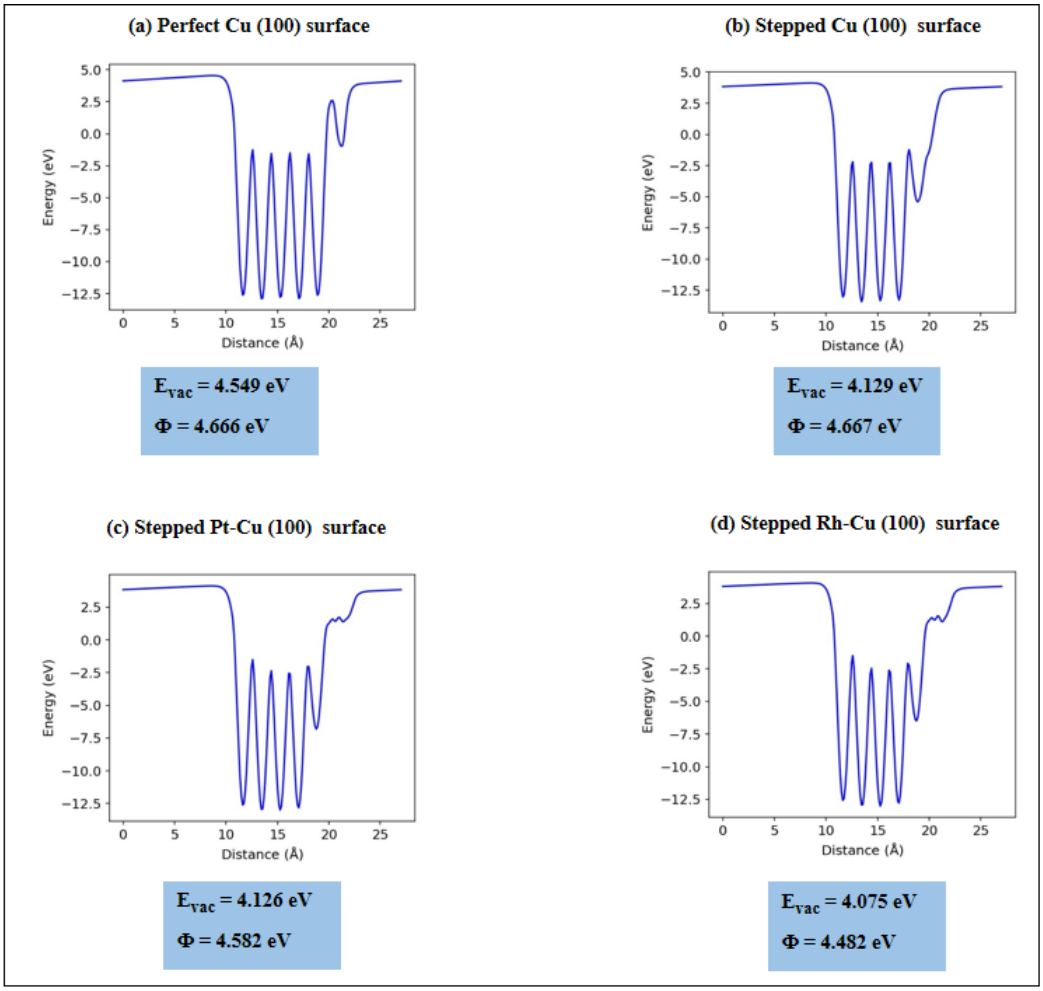

Figure S3: Planar-averaged electrostatic potential variation of adsorbed thiophene on the perfect and stepped Cu (100) surface.
The distance (Å) indicates the position of surface layers and thiophene molecule along the Z direction (vacuum direction).

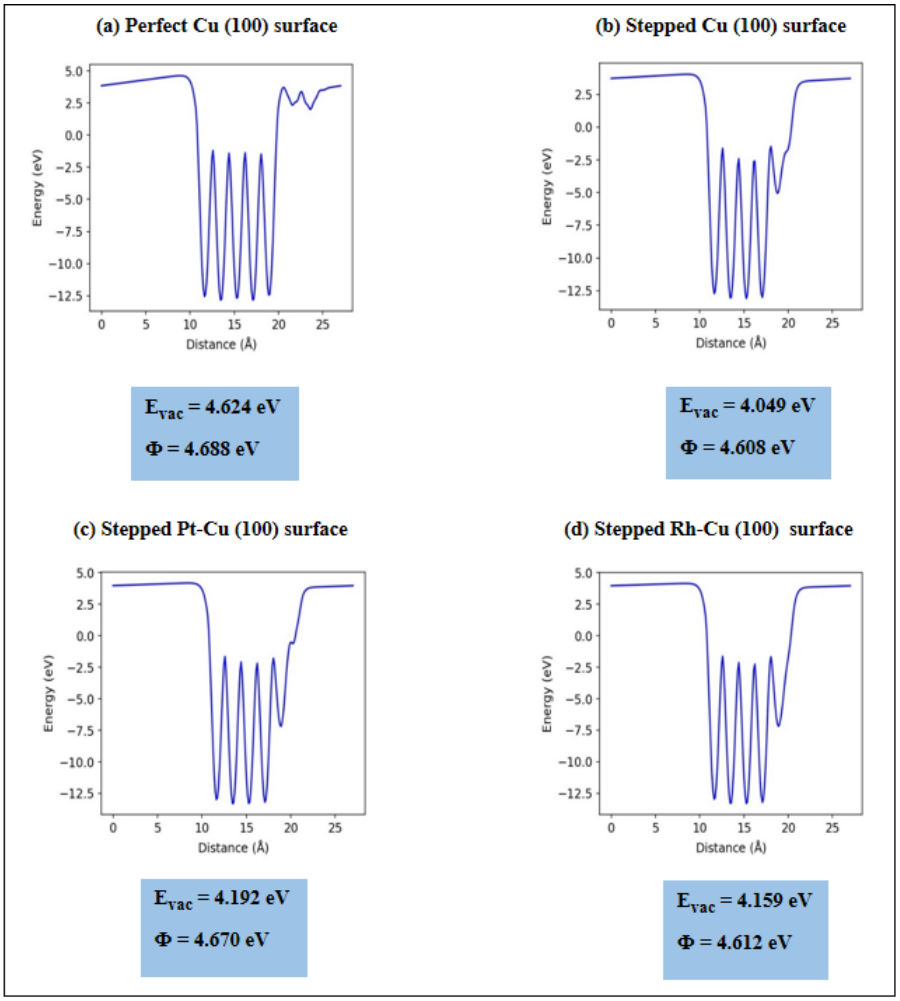

Figure S4: Planar-averaged electrostatic potential variation of adsorbed pyridine on the perfect and stepped Cu (100) surface.
The distance (Å) indicates the position of surface layers and pyridine molecule along the Z direction (vacuum direction).

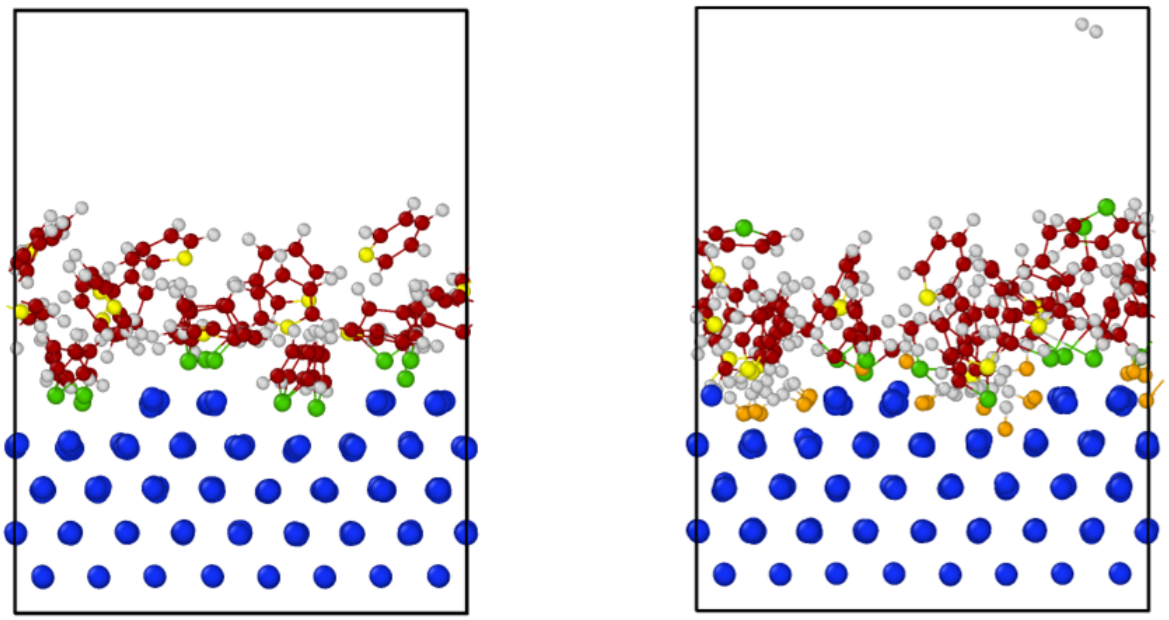

Figure S5: Full system of mixed adsorbate with (right) and without (left) water molecules. Blue, green, white, yellow, orange, and dark red balls represent Cu, S, H, N, O, and C atoms, respectively.

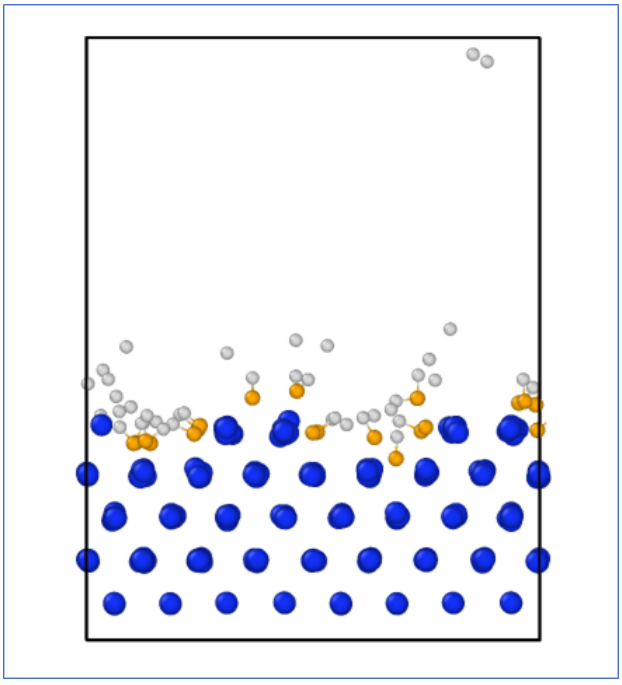

Figure S6: Water molecules adsorbed on Cu (100) stepped surface. Blue, white, and orange balls represent Cu, H, and O respectively.