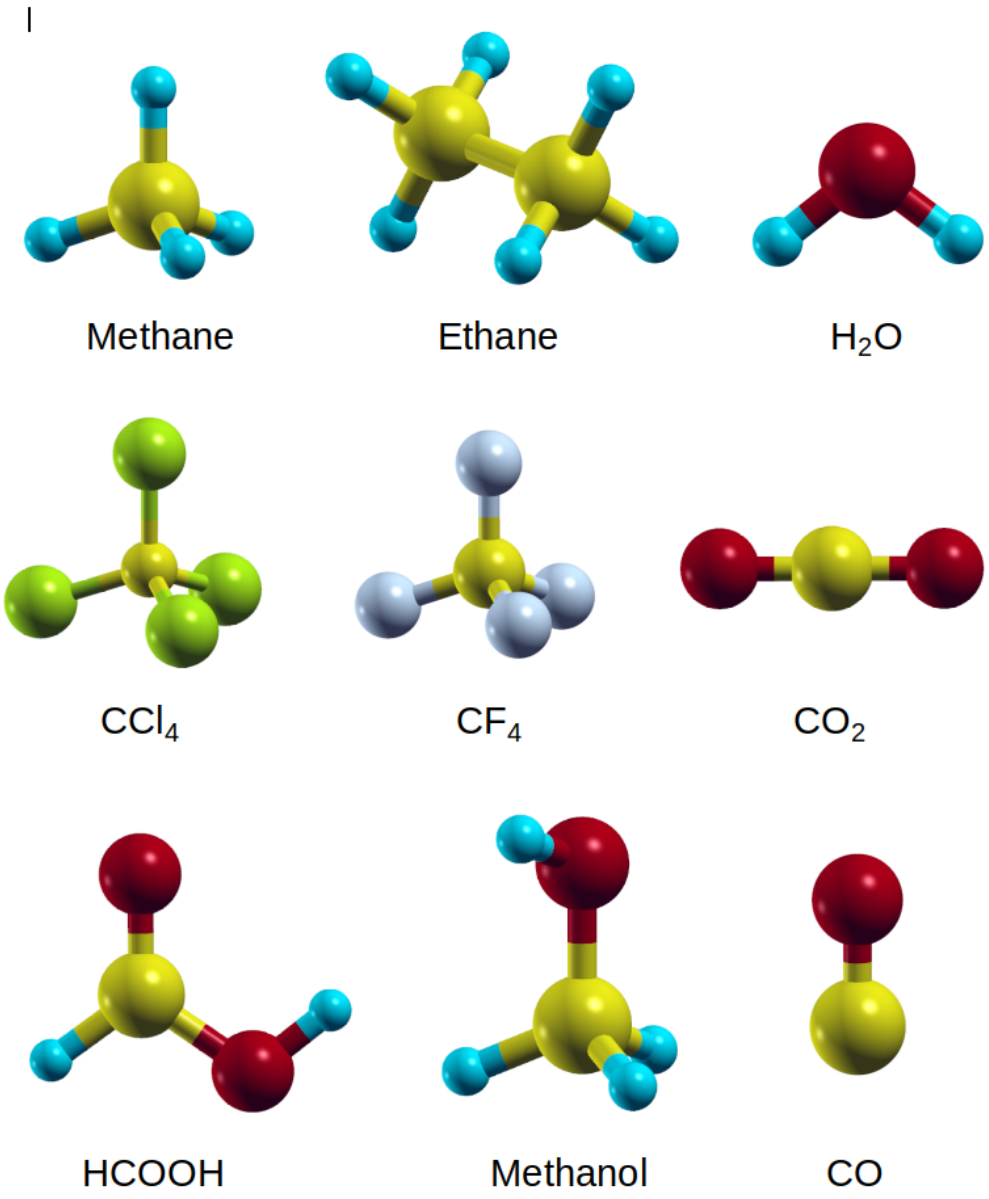
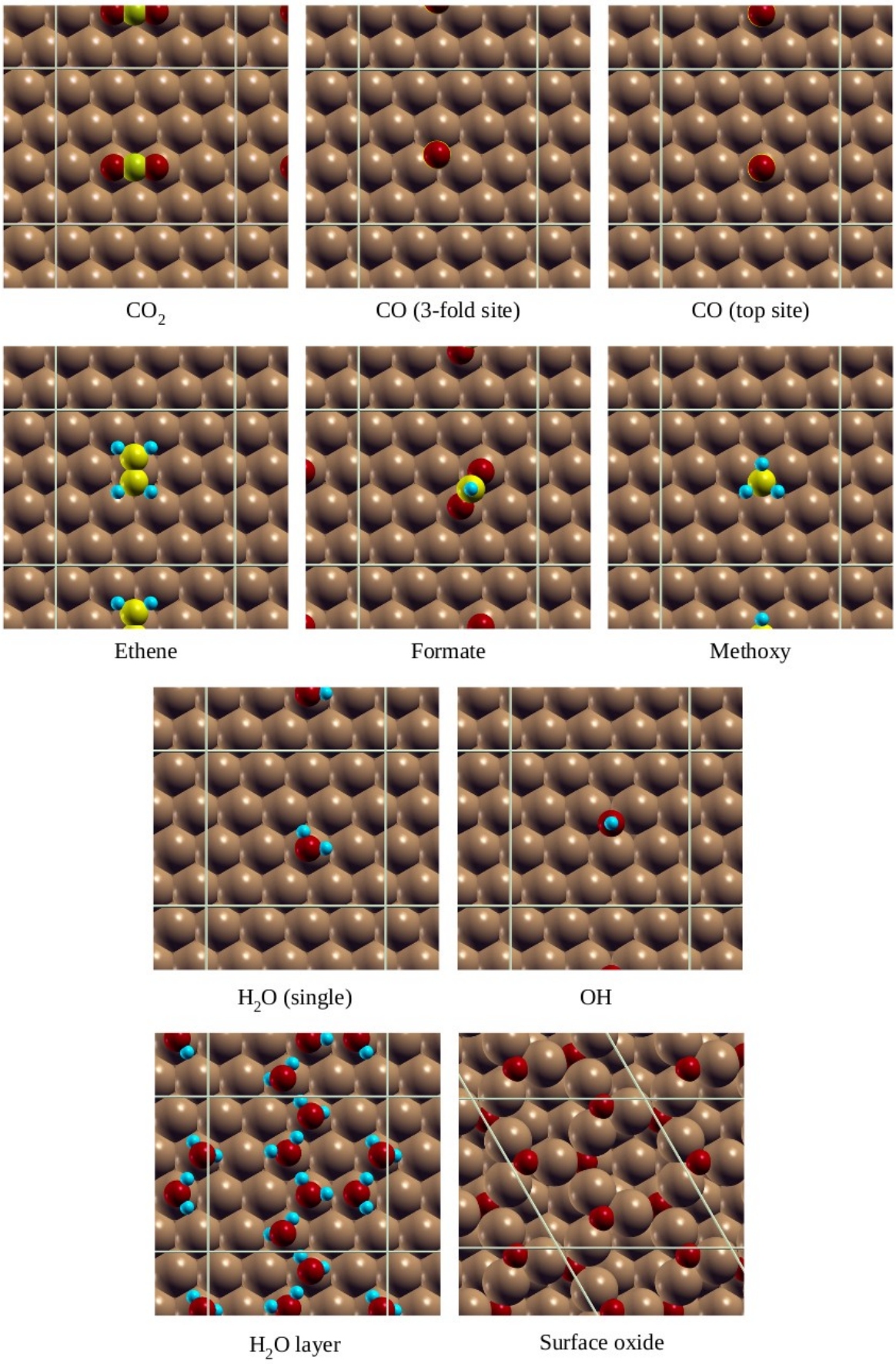
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.



Supplementary Figure 1: The geometries of the molecules used in the calculations of C1s and O1s core level binding energy shifts in gas phase XPS.



Supplementary Figure 2: The relaxed geometries of the adsorbates on Cu(111) slabs.