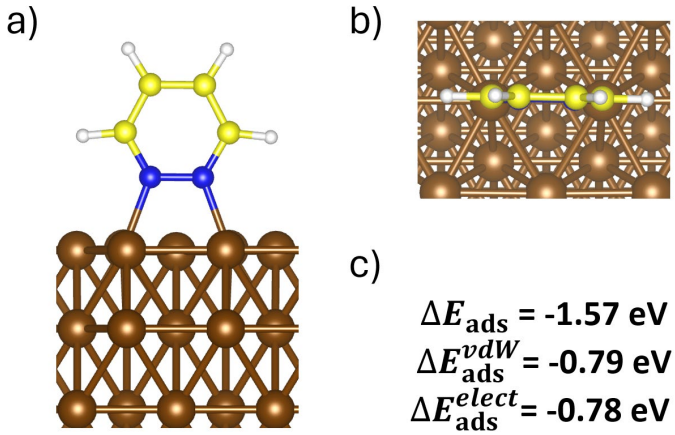

Figure 1: a) side, and b) top view representations of optimized pyridazine molecule on Cu (111) surface. c) total adsorption energy of pyridazine on Cu(111) surface and its electronic and dispersion components.

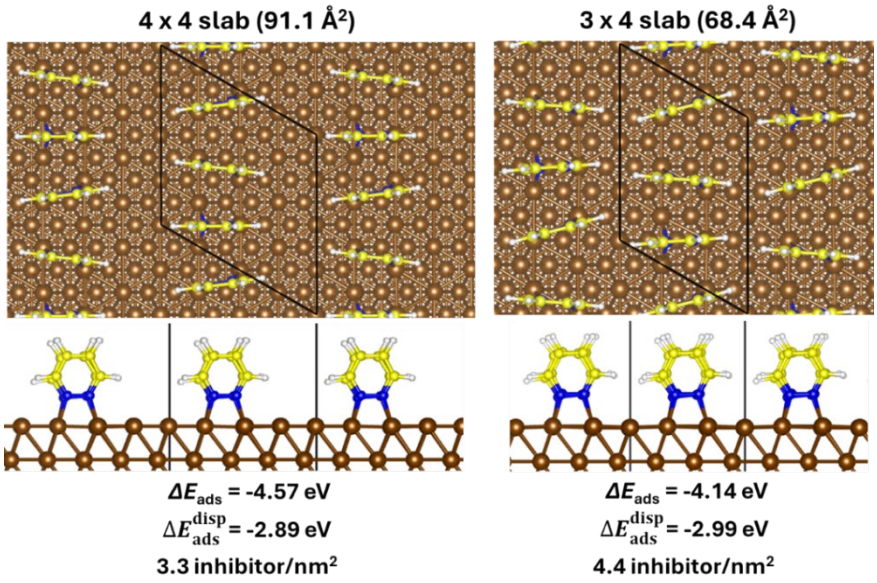

Figure 2: Top and side views of 4 x 4 and 3 x 4 supercells of Cu (111) surface saturated with pyridazine molecules. In ideal case, pyridazine molecules can favorably adsorb on Cu surface up to 4.4 molecules per nm^2. In real conditions, it is expected to observe a surface saturation density between RSA and DFT calculated values.

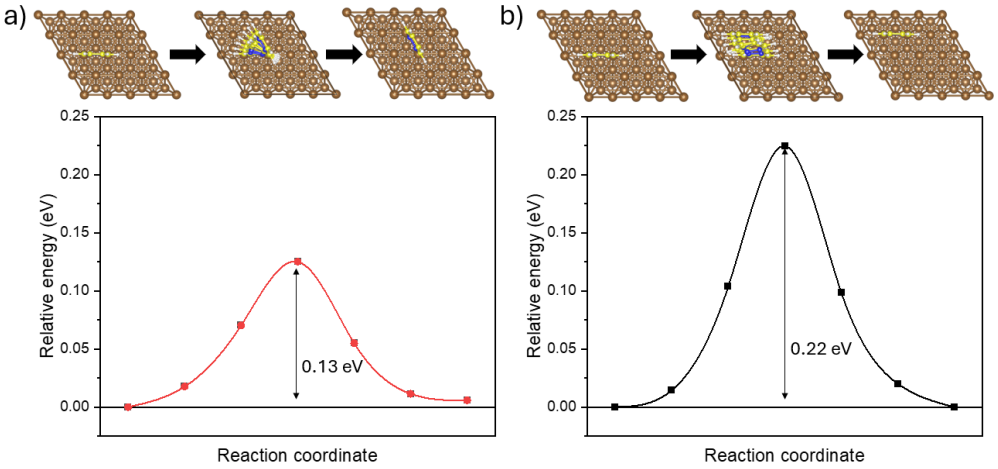

Figure 3: a) Rotation and b) diffusion of pyridazine on Cu (111) surface