Supplementary material for B806501B

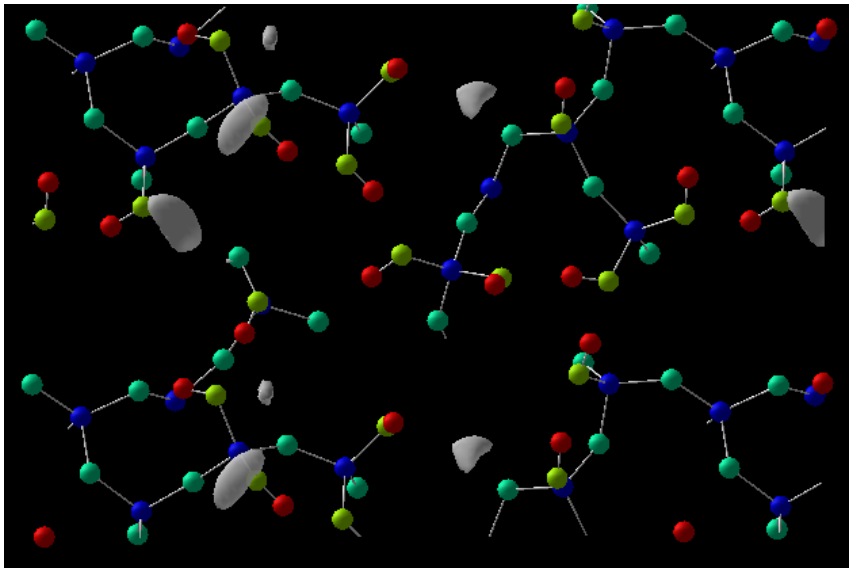
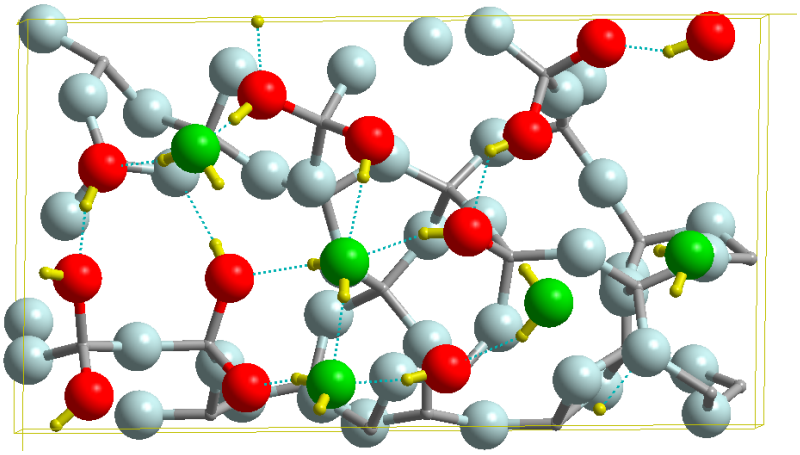
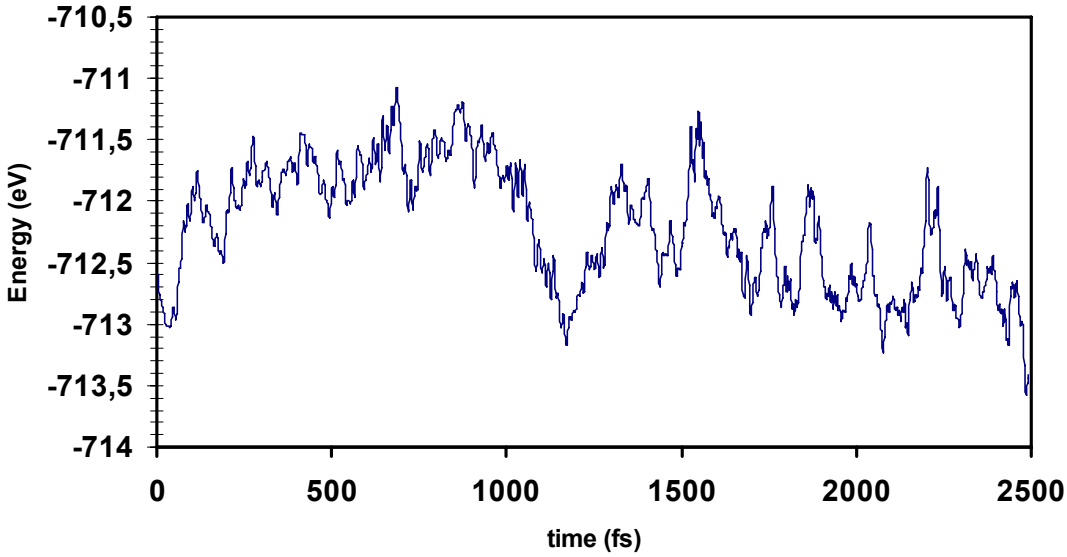


Figure 1: Electrostatic potential isosurface of -4eV of the studied amorphous silica surface. (Top view: H: red, Si: blue, O: green and yellow). One can clearly notice that the most negative zones of the electrostatic potential (nucleophile/electron donor zone) appears around the vicinal silanols of the hydroxylated silica surface.

a/



b/



c/

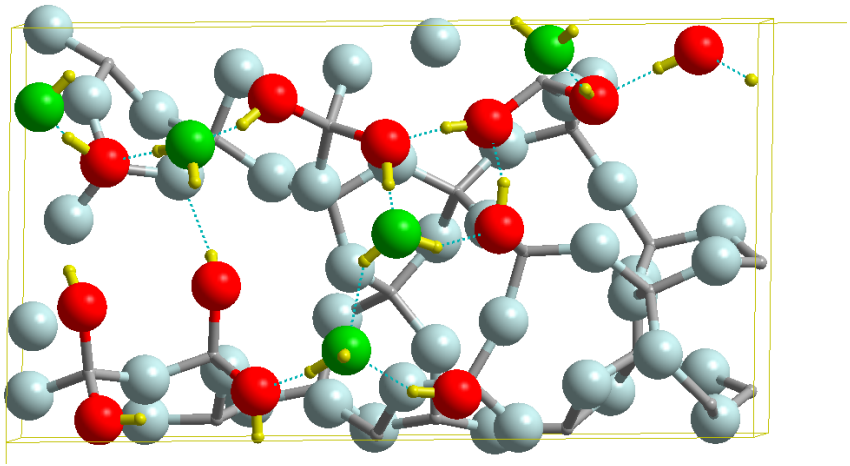


Figure 2 : MD run at 300K of five water molecules in interaction with the hydroxylated silica surface. a/ starting configuration, b/ energy versus time of simulation, c/ final configuration. Green: Oxygen of water molecules; Red: Oxygen of silanol, Large light gray: Oxygen in siloxane bridge, small dark grey: Si atoms.

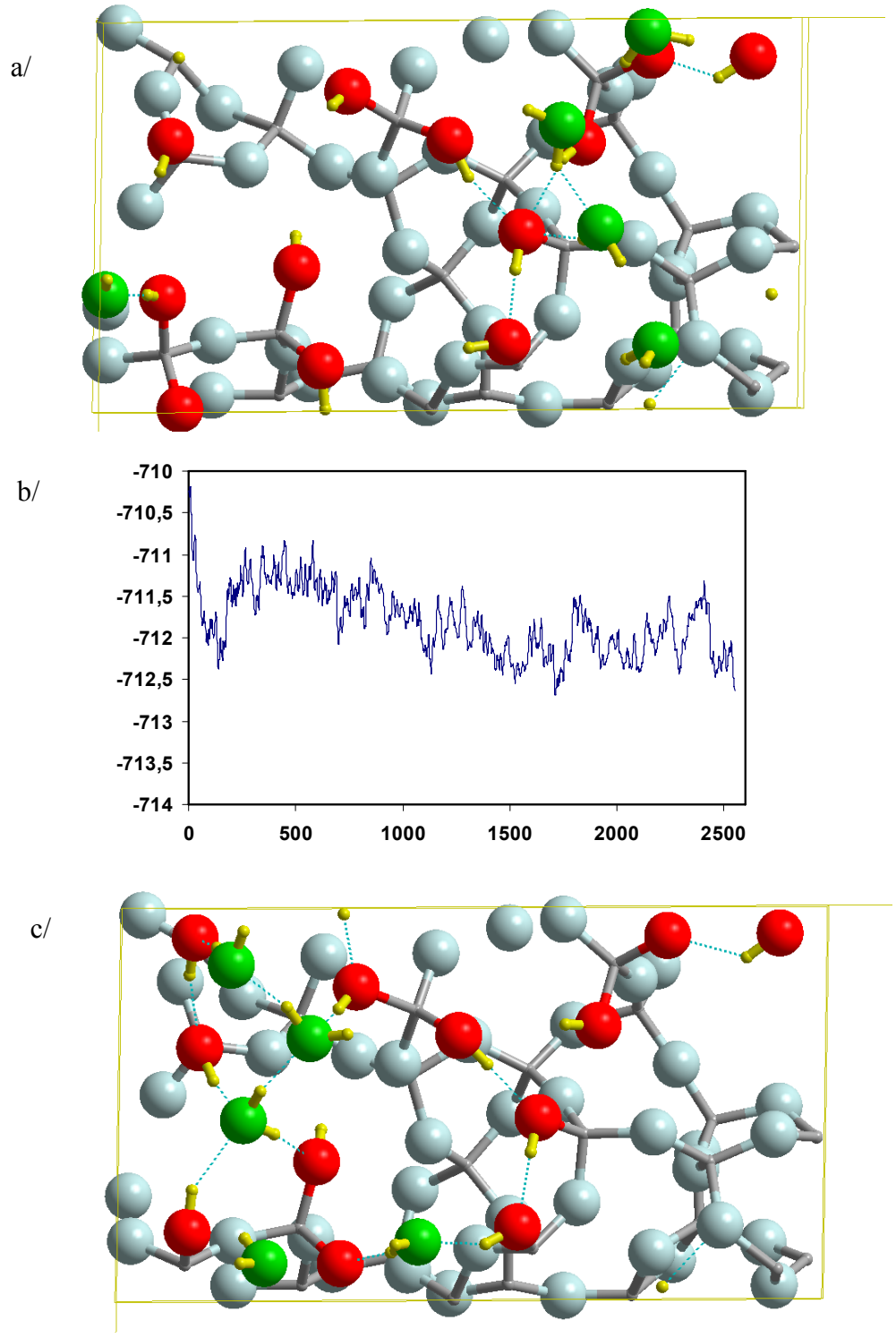
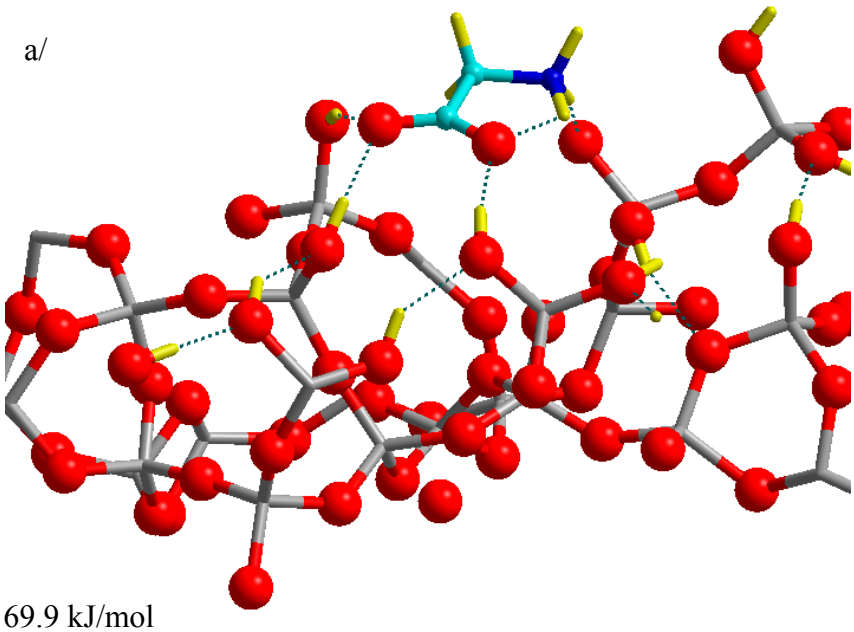


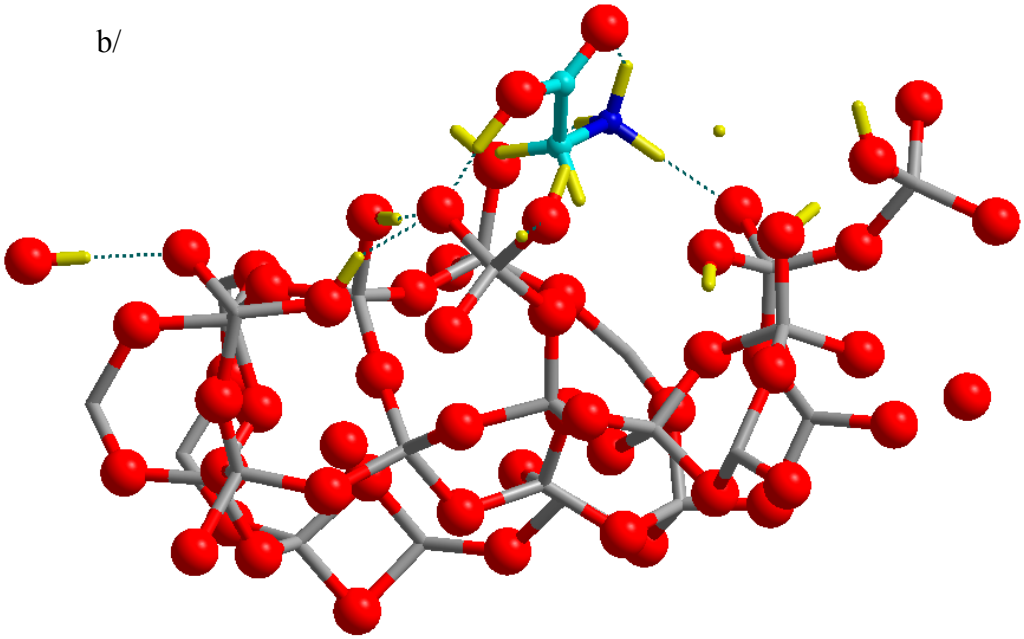
Figure 3 : MD run at 300K of five water molecules in interaction with the hydroxylated silica surface. a/ starting configuration, b/ energy versus time of simulation, c/ configuration at a local minimum at the end of the simulation. Green: Oxygen of water molecules; Red: Oxygen of silanol, Large light gray: Oxygen in siloxane bridge, small dark grey: Si atoms.

a/



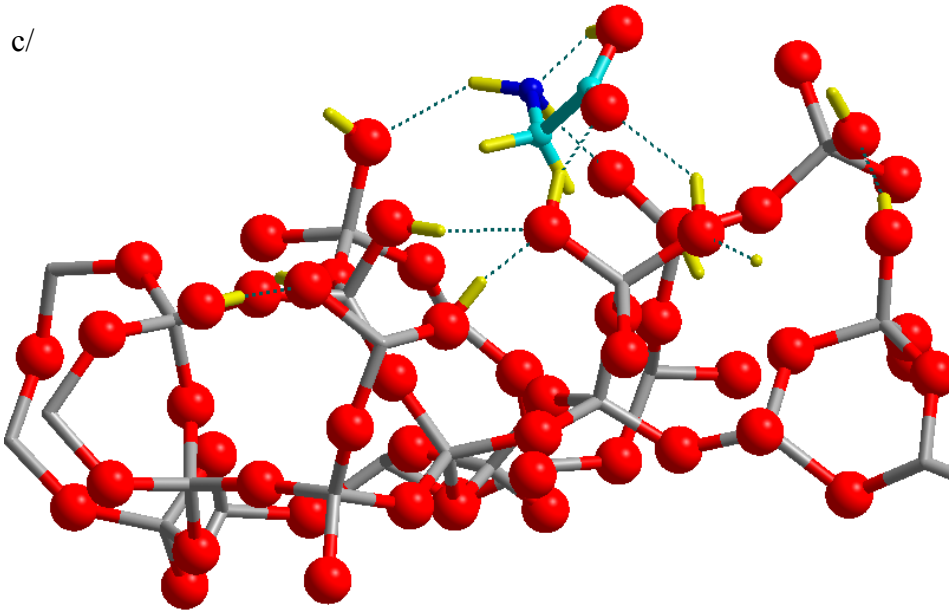
E_{ads} = - 169.9 kJ/mol

b/



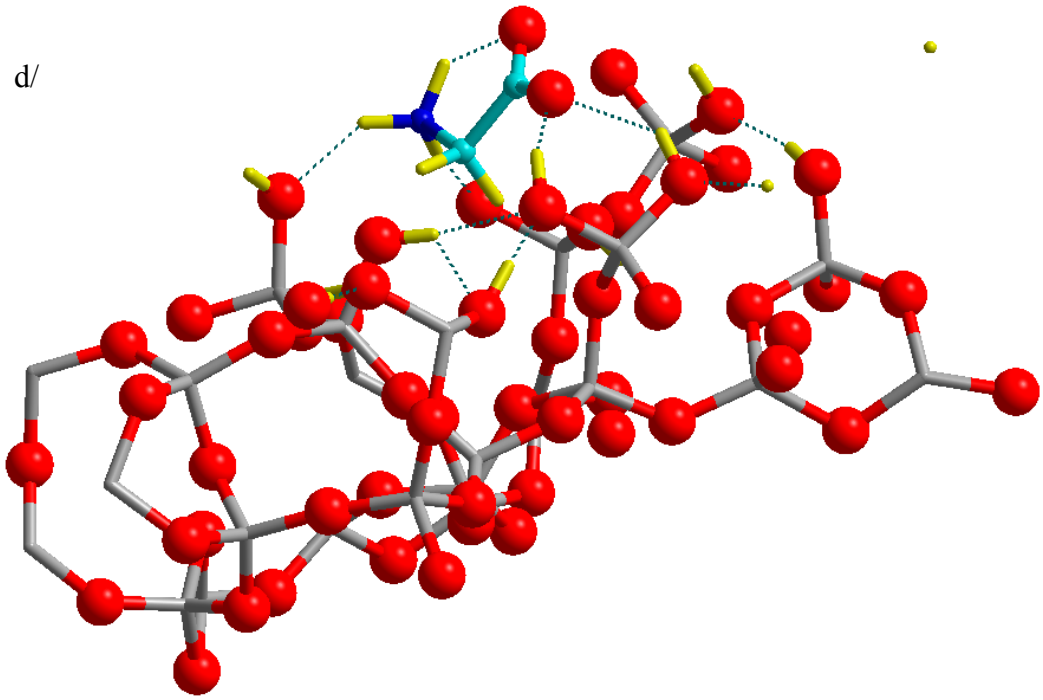
E_{ads} = - 163.2 kJ/mol

c/



E_{ads} = -136.2 kJ/mol

d/



E_{ads} = -102.4 kJ/mol

Figure 4 : Optimized geometries of glycine in several conformations on the hydroxylated silica surface.