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.
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.
E_{ads} = -169.9 \text{ kJ/mol}

E_{ads} = -163.2 \text{ kJ/mol}
Figure 4: Optimized geometries of glycine in several conformations on the hydroxylated silica surface.

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E_{\text{ads}} = -136.2 \text{ kJ/mol}
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\[
E_{\text{ads}} = -102.4 \text{ kJ/mol}
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