Investigating the Adsorption Mechanism of Glycine in Comparison of Catechol on Cristobalite Surface Using Density Functional Theory for Bio adhesive Materials

Shabeer Ahmad Mian[a, b*], Younas Khan[a], Uzair Ahmad[b], Mohammad Adil Khan[b], Gul Rahman[c], Shahid Ali[a]

[a]Department of Physics, University of Peshawar, 25120 Peshawar, Pakistan

[b]Department of Physics, Islamia College Peshawar, 25120 Peshawar, Pakistan

[c]Institute of Chemical Sciences, University of Peshawar, 25120 Peshawar, Pakistan

Electronic Supplementary Information (ESI)

In marine environment the mussels are surrounded by water and the same for the protein it secreted to adhere to the rocks. In order to mimic this wet environment we first model the water molecule for its adsorption on cristobalite surface. The water molecules and cristobalite surface were optimized before their interaction with each other. The same process was done for the catechol and water and cristobalite surface previously published[14-16]. Initially we perform the dry adhesion of glycine on cristobalite surface in order to compare with the catechol adsorption on dry surface. The reason for doing such an adsorption is to first confirm the dry adhesion and their comparative strength. The wet environment we actually introduce in the next step in order to develop more interest of the readers.

We introduce the reaction solvation method to observe the bond strength of glycine and water on hydrophilic surface. To do so we consider five water molecule on the cristobalite surface and also the co-adsorption of water molecule with glycine amino acid on the same surface. We optimized the geometries of both molecules and surface separately. The optimized geometries

were considered in such a way that the glycine is surrounded by five water on the cristobalite surface. It is much clear from the graphical representation of figure S1 that the five water molecule surround the adsorbed glycine on cristobalite surface. It is observed that bonding sites of adsorbed glycine but it does not affect the. On the dry cristobalite surface the glycine make 4 hydrogen bonds with the surface silanols and one hydrogen bonds with in the glycine carboxylic and ammonia part. On the wet surface glycine make 4 hydrogen bonds with surface silanols while two hydrogen bonds with the water molecule.

The glycine is rotated from the plane by approximately 60° and move towards the corner silanols forming the same four hydrogen bonds with the surface silanols. In the case of dry adsorption of glycine on the surface the average hydrogen bond length is approximately 1.768 Å but after the addition of five water molecules adsorption the average hydrogen bond length with surface silanols become 1.685 Å. In addition to these four hydrogen with surface silanols glycine carboxylic and ammonia part make two hydrogen bonds with surface. This way glycine make total of six hydrogen bonds with the surface and surrounded water molecules. This indicates that introducing of water medium to the glycine adsorption further strengthen the binding of glycine to the cristobalite surface.

In figure S1 the bonding of glycine with surface silanols and water is clearly shown to understand the adsorption mechanism. All the optimized geometries of five water molecules co-adsorbed with the glycine on the cristobalite surface, five water molecules adsorbed on the surface, five water molecule and five water molecules along with glycine are given in figure S1, S2, S3 and S4 respectively.
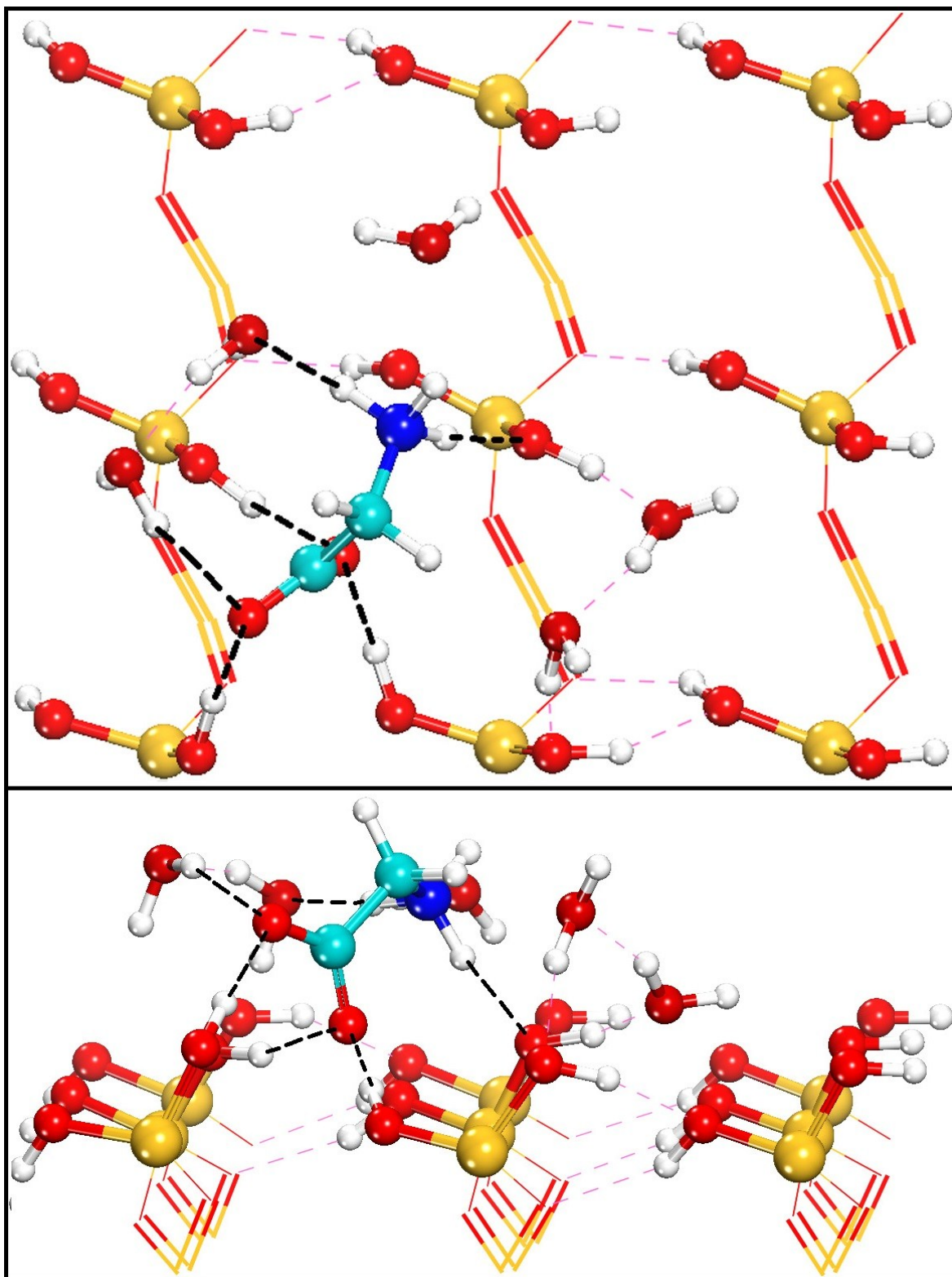
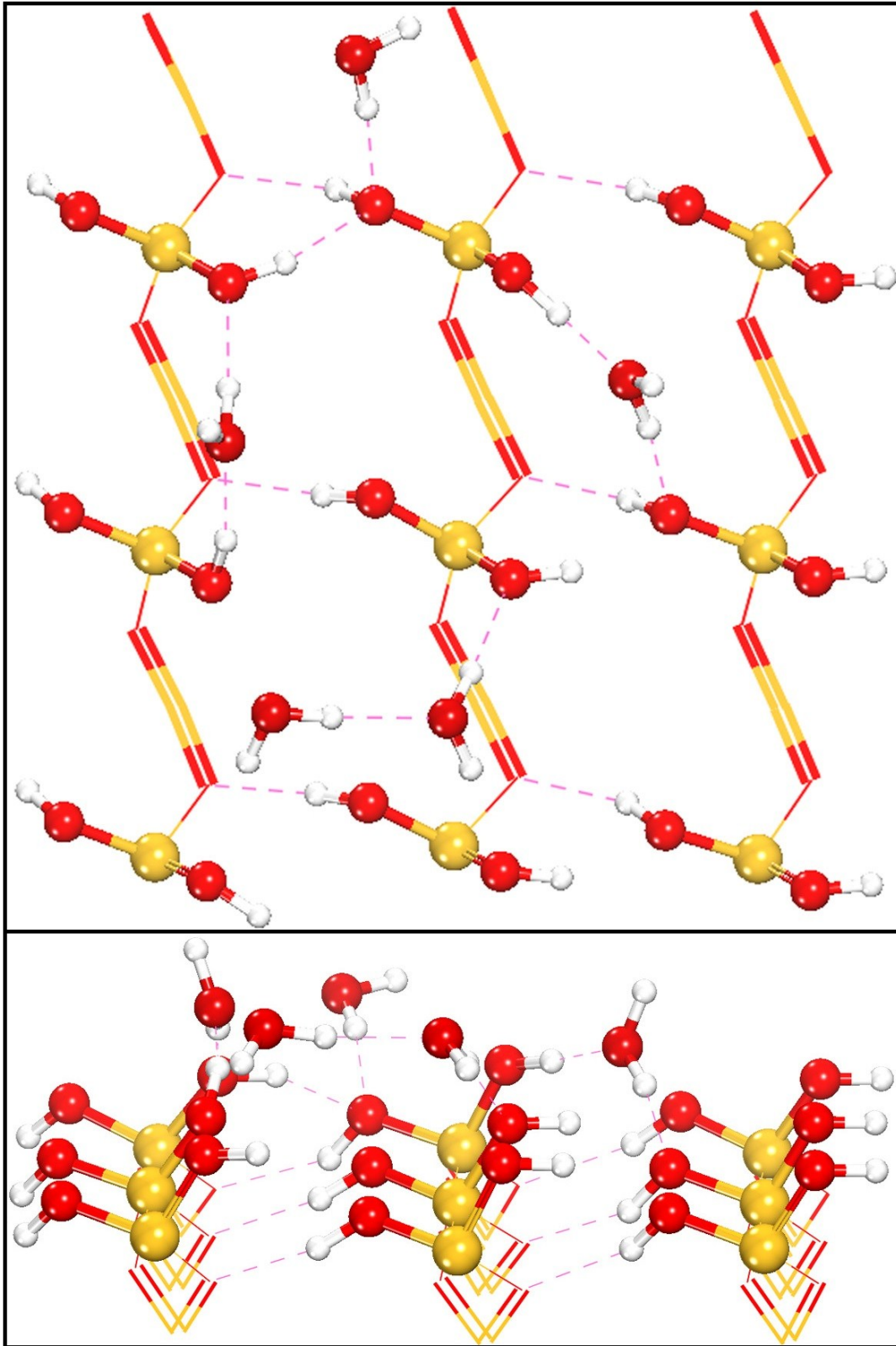**Figure S1:** Water Glycine co-adsorbed on Cristobalite surface

Figure S2: Optimized geometry of five Water molecule adsorbed on Cristobalite surface
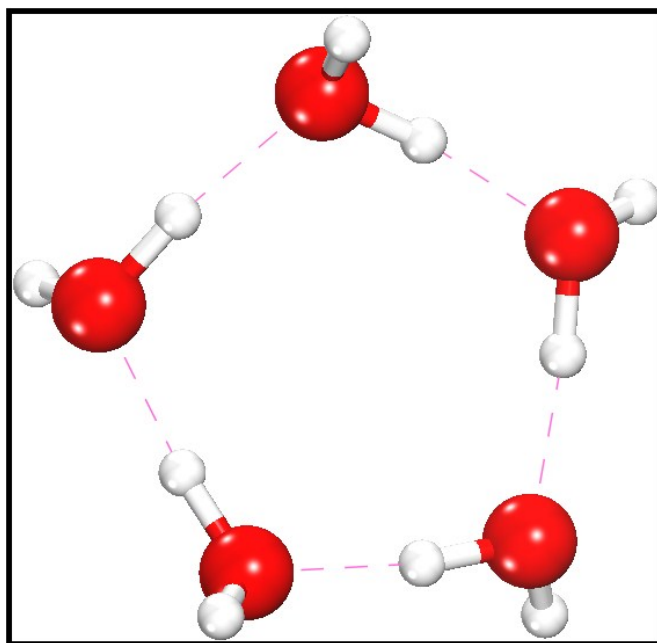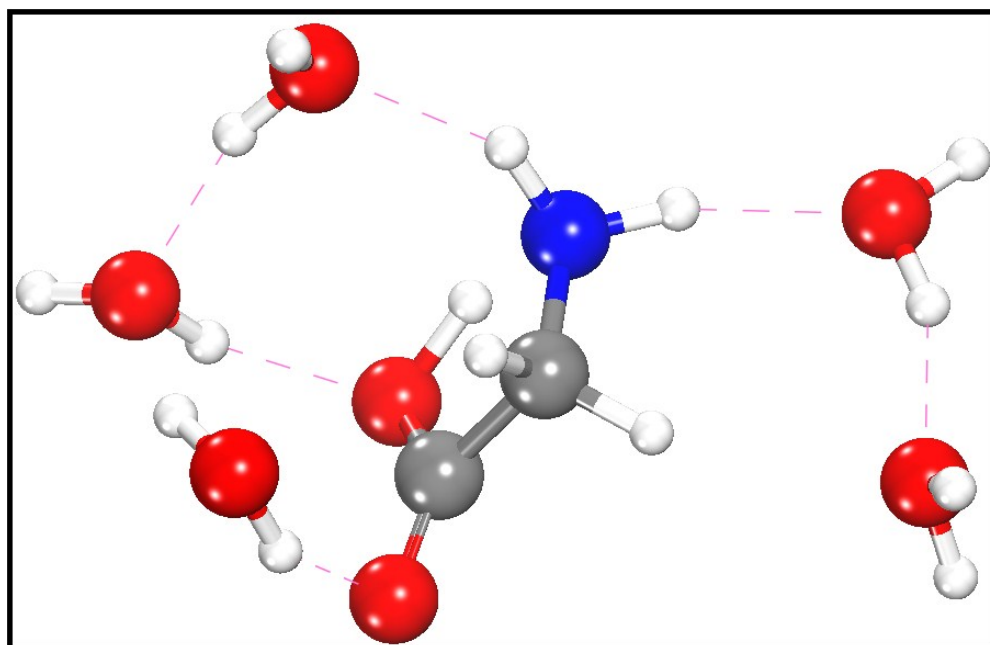
Figure S3: Optimized Geometry of five Water molecule

Figure S4: Optimized combine Geometry of Water Glycine