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Interactions between glucosides of the tip of the S1 subunit of SARS-CoV-2 spike protein and dry and wet surfaces of CuO and Cu—A model for the surfaces of coinage metals

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ABSTRACT

Despite their importance there is little knowledge at the atomic scale on the interactions between fragments of SARS-CoV-2 and inorganic materials. Such knowledge is important to understand the survival of the virus at surfaces and for the development of antiviral materials. Here is reported a study of the interactions between glucoside monomers of the tip of the S1 subunit of SARS-CoV-2 spike protein with dry and wet surfaces of CuO and Cu, performed with dispersion corrected density functional theory—DFT. The three glucoside monomers that constitute the tip of S1: 6VSB, 6VXX and 6X6P, were adsorbed onto dry and wet CuO(111) and Cu(110) with different orientations and surface alignments. There are large differences—of up to 1.3 eV—in binding energies between these monomers and the surfaces. These differences depend on: the type of surface; if the surface is wet or dry; if the glucosidic O-atom points towards or away from the surfaces; and to a smaller extent on the surface alignment of the monomers. All monomers bind strongly to the surfaces via molecular adsorption that does not involve bond breaking in the monomers at this stage. 6VSB has the larger adsorption energies—up to 2.2 eV—due to its larger dipole moment. Both materials bind the monomers more strongly when their surfaces are dry. At Cu(110) the bonds are on average 1 eV stronger when the surface is dry compared to wet. The difference between dry and wet CuO(111) is smaller, in the order of 0.2 eV. Overall, it is here shown that the stability of the monomers of the tip of the spike protein of the virus is very different at different surfaces. For a given surface the larger binding energies in dry conditions could explain the differences in the surface stability of the spike protein depending on the presence of moisture.

1. Introduction

COVID-19 the disease caused by the coronavirus SARS-CoV-2 is an emergency that has caused enormous damages to mankind. Roughly one year after the first reported global cases, a great deal of knowledge about the virus responsible for the disease has been gathered. However, to this date, there are still many unknowns regarding the survival of the virus outside the human body, especially at the inorganic surfaces that constitute the world around us. Some reports claim that this virus, as previously found for other coronaviruses [1], has the ability to survive on surfaces for hours or even days [2] while other reports claim that the viral RNA found on surfaces are only dispersed fragments and thus not able to infect living organisms because these fragments are part of a virus that has been damaged and as such inactivated [3]. Based on the current knowledge on how different surfaces have very different ability to drive chemical processes, such observations will certainly, to a large extent, depend on the type of surface and its environment [4–10].

The rush for gaining knowledge on the agent that causes the disease has led to an array of important publications with details on the structure of the virus down to the range of the 10 Å [11]. While a lot of work has—fortunately—been done in this area, up to date there are only few accounts of studies that have focused on mechanistic details of the interactions of the virus with inorganic surfaces [12]. It is important to understand these interactions because such surfaces have the potential to act as virus reservoirs [1,2]. Knowing the atomic scale mechanisms behind these interactions is essential to develop better understanding of the physical-chemical properties of virus, to understand the performance of different modeling methods and can guide the design of effective antiviral surfaces and coatings.

Because the interactions of most organic matter with inorganic...
surfaces are largely controlled by anisotropic dispersion forces [13,14], the challenge of understanding the details of the interactions between the virus with these surfaces is enormous. This is a task not easily at reach of current experimental methods, and the computational methods purely based on classical force-fields fail to account properly for those forces. This is because of the lack of accurate parameters for such a heterogeneous system—consisting of the inorganic components: metals, oxides, etc; in contact with organic matter, the virus. The solution to this problem is then to model the system with modeling tools based on quantum mechanics. But because employing high level quantum mechanical computations to the whole virus—or even to large pieces—is not at reach of our current computational tools, the challenge here is to find suitable models and computational tools that can be used to model important parts of the system virus-surfaces with good accuracy.

Studies on the virus structure have shown that the spike proteins located at the surface of the virus are important mediators of the interactions between the virus and its environment [15]. The tip of the spike proteins of the intact virus is composed of the so-called subunit S1 [11]. This subunit is in turn connected to the subunit S2. S1 acts as a sensor for the medium and can transmit that information either to S2 via a series of structural and chemical changes that occur at the interface between S1 and S2 [11]. Among other things this process mediates the entry of the virus into cells [16,17] and the S1 subunit is the target of an array of vaccine concepts [18–20]. At the tip of S1 there are three monomers of glucosides [11,15]. The detailed structures of those monomers have been published and have the PDB identities 6VSB [21], 6VXX [22], and 6X6P [23]. Because these monomers are the contact points between the virus and the environment, understanding their interactions with inorganic surfaces can give important mechanistic information on how such surfaces may affect the virus.

Coinage metals, the elements from group 11 in the periodic table, are important materials in our daily life, for which copper is often used as a sensor for the medium and can transmit that information to S2 via a series of structural and chemical changes that occur at the interface between S1 and S2 [11]. Among other things this process mediates the entry of the virus into cells [16,17] and the S1 subunit is the target of an array of vaccine concepts [18–20]. At the tip of S1 there are three monomers of glucosides [11,15]. The detailed structures of those monomers have been published and have the PDB identities 6VSB [21], 6VXX [22], and 6X6P [23]. Because these monomers are the contact points between the virus and the environment, understanding their interactions with inorganic surfaces can give important mechanistic information on how such surfaces may affect the virus.

The electronic structure calculation methods here employed have been previously extensively tested and benchmarked in varied studies of adsorption on pure and oxidized Cu surfaces as well as hydroxylated Cu surfaces [37–39]. DFT calculations were performed with the Vienna ab initio simulation package [40] (VASP 5.4.4) employing the exchange-correlation functional by Perdew-Burke-Ernzerhof, PBE (Refs [41,42]) with pseudopotentials of the projector augmented wave [43,44] (PAW) type which are coherent with the ultrasoft type. The van der Waals interactions which are important for the correct description of the structure of hydrogen bonded structures [45–47] were described with the zero damping D3 correction [48] by Grimme as implemented in VASP. The PBE functional with corrections of the D type has shown good performance for modeling complex hydrogen bonded structures and for the description of adsorption and desorption in structures dominated by H-bonds [45,47]. For the geometry optimizations and single point energy calculations, a plane wave cutoff energy of 560 eV and a k-point mesh of (2 × 2 × 1) in the Monkhorst-Pack sampling scheme [49] were used together with Gaussian smearing with a width of 0.05 eV.

Stoichiometric monoclinic CuO(111) [50], and fcc Cu(110), were simulated with periodically repeating slabs in supercells with surface symmetries p3×2 and p3(3×3) respectively, and vacuum thicknesses of 15 Å and 25 Å respectively. For CuO(111), the slab consisted of 128 atoms with a thickness of 2 stoichiometric unit cells of CuO. For the geometry optimizations the bottom layer was constrained, and the remaining atoms were relaxed. The slab of Cu(110) consisted of 108 Cu-atoms disposed in 3 layers where the bottom layer was constrained and the remaining atoms were relaxed. To model the wet surfaces, both surfaces were hydrated-hydroxylated according to the literature knowledge for when these materials are exposed to a water containing environment, such as moisty air [30,37]. The adsorption energies (ΔEads) reported herein have been determined as

\[ \Delta E_{\text{ads}} = E_{\text{product}} - \sum E_{\text{reactants}} \]

where \( E_{\text{product}} \) represents the electronic energy of the adsorbate bound to the slab and \( E_{\text{reactants}} \) represents the electronic energy of the bare slab and that of the adsorbate in gas-phase. A more negative value for \( \Delta E_{\text{ads}} \) implies stronger adsorption.

The glucoside monomers of the tip of the subunit S1 of the SARS-CoV-2 spike protein: 6VSB [21], 6VXX [22], and 6X6P [23], were retrieved from PDB. These monomers consist of isomers of 2-acetamido-2-deoxy-beta-D-glucopyranose. The retrieved conformations are the AA for every monomer and have been chosen in order to have monomers both in cis and in trans conformations. The monomers have been disposed at the surfaces one by one with their main axis parallel to each surface plane vector and in conformations in between. After this, a geometry optimization was performed where all atoms of the monomers and all atoms of the surface slabs except the bottom layer were allowed to relax. Only the most stable conformations obtained are here presented and discussed.
Solvation effects have been simulated with VASPsol which adds an implicit solvation model to VASP [51,52] and where water with a dielectric constant of 78.3 at 25 °C has been used. Test calculations for selected cases revealed that the solvation contribution to the adsorption energies varied from 0.08 eV for CuO(111) to 0.21 eV for Cu(110). The decrease of the adsorption energies is very small for all cases investigated due to the large magnitude of the adsorption energies in comparison with the contribution from the solvation effects. For molecular adsorption as studied here, the solvation energies of the fragments are close to constant during the reaction, as it has been previously observed for H₂O [37]. The exception to this is the solvation at the interface between the fragments and the surfaces which has been here explicitly considered with wet surface models as detailed below. Because the interface solvation is the most relevant for the interactions between the viruses and surfaces [53] and given that the contribution of the solvation is very small in comparison with the adsorption energies, and due to some limitations of the solvation model for describing adsorption [54], the effects of implicit solvation have not been included in this work.

3. Results and discussion

3.1. Dry and wet CuO(111) and Cu(110)

The bare wet surfaces of CuO and Cu were prepared for the study of adsorption of the glucoside monomers by the subsequent creation of 1 ML of adsorbed H₂O on the initially dry surfaces, generating structures similar to those reported in previous works [30,37–39]. The difference between the current case and the cited works is that significantly larger supercells are here employed. The perfect Cu(110) surface can be used to simulate molecular adsorption onto real Cu surfaces with good accuracy because it contains 5 symmetrically non-equivalent binding sites [38]. These different coordination sites can to a good extent mimic the role of some point defects in molecular adsorption [39,55]. At the CuO(111) surface, point defects at room temperature have a smaller role in molecular adsorption because of the ionic nature of the bonding at the surface and its ease in relaxing, reconstructing and annihilating some of the defects [56].

Upon exposure of the dry surfaces to ambient air containing considerable moisture it is likely that additional MLs of H₂O form. However, the H₂O molecules at MLs far from the surface are not as relevant for the adsorption of the glucosides as the first ML of H₂O—the closest to the surfaces. This is because the bonds between H₂O and the surfaces are considerably stronger for the first ML and the H₂O in higher MLs are bound via H-bonds with similar strengths to those in liquid water [37]. The dry and wet surfaces are shown in Fig. 1. For Cu(110), the first ML of adsorbed water consists of alternating HO and H₂O along both directions A and B according to a previously reported structure [37]. For CuO(111), the surface here considered is fully covered with water, 1 ML, where the bound H₂O forms a pattern containing ½ ML of HO and ½ ML of H₂O [30]. According to previous studies, in the lowest energy structure, these adsorbates are disposed in alternating rows of HO and H₂O, along the B direction. This was also observed in this study.

![Fig. 1. Dry and wet surfaces of Cu(110) and CuO(111) employed in the study of the adsorption of the glucoside monomers. The axes A and B correspond to the following directions: A = [001], B = [110] in Cu(110); and A = [001], B = [011], in CuO(111). The black lines show the supercells. The bottom figures show the alignments of a glucoside relative to the axes A and B of the surfaces. These two alignments are designated by A and B, respectively. Cu (●), O ( ○), H (○).](image-url)
and can be seen in Fig. 1.

The $\Delta E_{\text{ads}}$ values obtained for the molecular adsorption of 1 H₂O are in excellent agreement with previously published data: $\Delta E_{\text{ads}}$ (CuO) $\approx$ −0.24 eV for the hollow site and −0.19 eV for the ridge; \(^{24}\) $\Delta E_{\text{ads}}$ (Cu) $\approx$ −0.25 eV \(^{55}\). The values obtained for 1 ML are also in very good agreement with literature data \(^{37}\).

3.2. The glucoside monomers 6VSB, 6VXX and 6X6P

The structures of the glucoside monomers 6VSB, 6VXX and 6X6P in gas-phase were optimized starting from the PDB data with subsequent hydrogenation according to the known coordination rules for carbohydrates \(^{57,58}\), leading to neutral molecules with singlet spin. No considerable changes to the structures have occurred upon geometry optimization with PBE-D3 which shows the good accuracy of the method for the structural modeling of these molecules. The resulting structures are shown in Fig. 2.

3.3. Interactions of 6VSB, 6VXX and 6X6P with dry and wet CuO(111) and Cu(110)

The monomers shown in Fig. 2 were placed at the surfaces in different orientations with the glucosidic O-atom (double bonded) pointing up as shown in the right-hand side panels of Fig. 2 or flipped with this O-atom pointing down towards the surface. For simplicity, these two orientations will respectively be referred to U and D from onwards. Additionally, the adsorption geometries of the monomers are labeled A, or B depending on the alignment between the monomer and the surface axes upon adsorption as shown in Fig. 1. The resulting structures are shown in Figs. 3 and 4 for CuO and Figs. 5 and 6 for Cu. The corresponding adsorption energies are shown in Figs. 7 and 8.

Figs. 3–6 show that the bonding between the glucoses and the surfaces occurs in two ways: via O-atoms (the glucosidic O-atom and alcohol O-atoms); and via H-atoms. This shows, contrary to what has been previously speculated, that van der Waals interactions play an important role in the adhesion of the virus to surfaces \(^{59,60}\). It is now widely known that van der Waals forces are present in both of these types of interactions with the surfaces, bonding via O and H-atoms, but it is more significant in the formation of H-bonds with the surfaces as previously shown for similar systems \(^{37,61,62}\).

Due to its symmetry, the monomer 6VSB has both the glucosidic O-atom and the terminal alcohol O-atom pointing either towards the surface or away from it as shown in Fig. 2. While for the other two monomers either the glucosidic O-atom or the terminal alcohol O-atom point towards the surface. This leads to a larger dipole moment for 6VSB that affects both its $\Delta E_{\text{ads}}$ and adsorption geometry to very large extents. The result is that for the same surface, the $\Delta E_{\text{ads}}$ of 6VSB are considerably larger for all surfaces than for the other two monomers as shown in the data of Figs. 7 and 8. The exception to this is the wet Cu(110). A similar phenomenon has been previously observed for other adsorbates \(^{38}\). The increase in $\Delta E_{\text{ads}}$ happens because adsorbates with larger dipole moments induce also larger dipoles at the surface binding site and this increases their binding energy. Figs. 7 and 8 show also that the effect of the larger dipole in the adsorption energies of 6VSB is more pronounced for the dry surfaces. This is also in agreement with previous findings for other adsorbates. It is known that O-atoms bind stronger to Cu surfaces than H-atoms. This is also observed here for the studied monomers and causes a large dispersion in their adsorption energies which depend on if the monomers are oriented so that their glucosidic O-atoms point towards or away the surfaces. The adsorption structures show that for the conformations that lead to strong interactions with the surfaces, the bonds with the monomers are of a magnitude that causes the outwards dislocation of Cu atoms, a typical phenomenon that accompanies the formation of strong bonds with surfaces. This type of relaxation has been previously observed in the study of adsorption of H₂O onto this Cu surface \(^{37}\). At the dry Cu(110), the Cu-atoms that bind directly with the glucosidic O-atoms of the fragments expand outwards and their bond distances with the second layer of Cu-atoms changes by as much as 11% when compared to their equilibrium positions. The Cu-atoms that bind with the H-atoms of the fragments expand their bond distances with the second layer of Cu-atoms by only 0.5%, and those that bind via dispersion forces with the alcohol O-atom of the fragments expand by 1.8%. On average the expansions induced by the fragments when the glucosidic O-atom is pointing towards the surface is 6.4% and when the glucosidic O-atom points away from the surface is 1.6%. These different relaxations are the result of different chemical bonds: the covalent type bonding with the glucosidic O-atom; and the bonding with H-atoms and the OH group due to dispersion forces. For the cases where strong bonds occur the monomers also suffer considerable structural changes that affect internal bond lengths and angles.

The adsorption data shows that both Cu(110) and CuO(111) bind the monomers stronger when the surfaces are dry, and also that for the same surface there are large differences in $\Delta E_{\text{ads}}$ depending on if the surface is dry or wet. This effect is especially evident for metallic Cu. As visible in Figs. 3–6, the reason for this is that the chemical environment of the surface changes drastically from dry to wet Cu(110), while the difference between dry and wet CuO(111) is smaller because the dry CuO (111) is also composed of O-atoms. The latter case leads to similar bonds between the monomers and either dry CuO(111) or wet CuO(111), while for Cu(110) the monomers bind via very different types of bonds depending on if the surface is dry or wet. For the dry surfaces, the larger standard deviations for $\Delta E_{\text{ads}}$ shown in the set of data of Fig. 8 highlight the fact that the bonding between the monomers and these surfaces is more sensitive to the orientation and conformation of the monomers. This is also expected according to previous finds for other molecules \(^{37}\) because the bonding between the monomers and the dry surfaces has a higher dependency on the surface sites—top, long bridge, short bridge, etc.—while for wet surfaces the bonding occurs via H-bonds with O-atoms. This type of environment is more flexible in terms of orientation of adsorbates and has more local minima in what concerns stable binding sites than for the case of dry surfaces.

Figs. 7 and 8 show that between the orientation of the monomers (U or D) and their alignment (A or B), the orientation is the factor that has the largest effect on $\Delta E_{\text{ads}}$. Again the dry surfaces are those where the orientation U or D has a larger effect on $\Delta E_{\text{ads}}$ with differences that can
Fig. 3. Adsorption geometries for the monomers 6VSB, 6VXX and 6X6P at dry CuO(111). The monomers are oriented as U or D and A or B (see beginning of Section 3.3 for explanation).
Fig. 4. Adsorption geometries for the monomers 6VSB, 6VXX and 6X6P at wet CuO(111). The monomers are oriented as U or D and A or B (see beginning of Section 3.3 for explanation).
Fig. 5. Adsorption geometries for the monomers 6VSB, 6VXX and 6X6P at dry Cu(110). The monomers are oriented as U or D and A or B (see beginning of Section 3.3 for explanation).
Fig. 6. Adsorption geometries for the monomers 6VSB, 6VXX and 6X6P at wet Cu(110). The monomers are oriented as U or D and A or B (see beginning of Section 3.3 for explanation).
The differences between the surfaces are much stronger than for the wet surfaces, especially for Cu viral particles between surfaces [53]. Overall, the adsorption energies of the virus at these surfaces as well as the transmission rate of faces and the virus are the most important parameters that determine the results [63,64]. In the first work cited, interactions of the virus with the copper surfaces were able to trigger the restructuring of the spike protein leading to loss of function. In the current case it is expected that some of the large binding energies between the glucoside monomers and the surfaces will also lead to similar effects. This can have repercussions on the structure of the virus adjacent to the monomers of the tip of S1 and will consequently have effects in subsequent sections of the tip of spike protein directly connected to these sections. This could explain the shorter survival times of the virus at dry surfaces when compared to wet surfaces [10]. These results agree also with previous observations that show that the solvation of the interface between surfaces and the virus are the most important parameter that determine the life-time of the virus at these surfaces as well as the transmission rate of viral particles between surfaces [53]. Overall, the adsorption energies of the monomers onto both the dry and the wet surfaces are larger than the typical solvation energies of sugar monomers [65,66]. This implies that energetically, the adsorption of the monomers to the wet surfaces could cause the desorption of H\textsubscript{2}O which would lead to direct bonds between the monomers and the surfaces—without the presence of interfacial H\textsubscript{2}O at the contact point between the monomer and the surface. This would cause much stronger interactions between the monomers and the surfaces as shown in Fig. 8, which could trigger the inactivation mechanism. In this sense the mechanism of viral inactivation could occur even in the presence of water but would be slowed down due to kinetics and not because it is energetically unfavorable. However, real life studies are necessary to confirm the statistical occurrence of these phenomena because as the complete sets of adsorption data and the standard deviations show, there are many local minima in terms of stable binding sites for the glucosides to form bonds with the surfaces.

Fig. 7. Adsorption energies for the monomers 6VSB, 6VXX and 6X6P at dry and wet surfaces of CuO(111) and Cu(110). The monomers are oriented as U or D and A or B (see beginning of Section 3.3 for explanation).

4. Conclusions

The interactions between glucoside monomers of the tip of the S1 subunit of SARS-CoV-2 spike protein and dry and wet surfaces of CuO and Cu were here studied with dispersion corrected DFT calculations. The three glucoside monomers that constitute the tip of the S1 subunit: 6VSB, 6VXX and 6X6P, were disposed at the dry and wet surfaces with different orientations and alignments. The very large differences in binding energies (adsorption energies) between these monomers and the surfaces are attributed to the type of surface, the presence of water, and to the orientation of the monomer—if the glucosidic O-atom points towards or away from the surfaces. Due to a larger dipole moment, the monomer 6VSB has considerably larger adsorption energies that can reach ~2.2 eV, but all three monomers bind to the surfaces with very large binding energies considering that the process is the molecular adsorption and does not involve bond breaking in the monomers at this stage. For the cases where the bonds with the surfaces are very strong the monomers are subject to considerable structural changes and in the case of Cu(110), the surface sites that bind to the glucosidic O-atom of the monomers are subject to considerable outward relaxation. Both materials bind the monomers present at the tip of the S1 group of the spike protein more strongly in dry conditions. For Cu(110), the whole set of data shows that the monomers bind to this surface on average 1 eV stronger when the surface is dry when compared to wet. The difference between the adsorption energies of CuO(111) is smaller, in the order of 0.2 eV. The adsorption energies of H\textsubscript{2}O onto these surfaces and the typical solvation energies of sugar monomers suggest that the stronger bonds between the monomers and the dry surfaces can be enough to displace water molecules from the interface and create direct contacts between the monomers and the surfaces. However, this process can be hindered by kinetic constraints.

Overall these results show that the stability of the different monomers present in tip of the spike protein of the virus is very different at different surfaces and these differences depend largely on if the surfaces are wet or dry. The very large binding energies between the glucoside monomers and the dry surfaces and the structural changes that the monomers suffer in those cases can possibly lead to restructuring of the spike protein and its loss of function as previously observed for other proteins.

CRediT authorship contribution statement

Cláudio M. Lousada: Conceptualized the work, performed the investigation and wrote the paper.
Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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