Nanoscience and Covid-19: MD simulations of the interaction of the SARS-CoV-2 virus with materials and chemical agents

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The novel coronavirus SARS-CoV-2 emerged in December 2019 as a human pathogen that causes the COVID-19 pandemic. From the point of view of NanoScience, this virus is an organic nanoparticle with a diameter of ~90 nm made by a vesicle-like envelope of proteins and lipids encapsulating the viral genetic material. The virion particle has a large protruding spike S glycoprotein (~24 nm long) that covers the viral particle and give its crown-like characteristic appearance (hence the latin name "corona"). During these two years of pandemic, a wealth of structural information about the viral nanoparticle has been accumulating, including detailed 3D images of the envelope, protein structures with atomistic-resolution and many other molecular and supramolecular details. In our group, we have been employing this information in order to develop models of the virus and its interaction with materials and chemicals, using molecular dynamics (atomistic and coarse-grain) simulation techniques. This is a topic of fundamental importance, given its role in virus transmission (filters, face masks, possible surface contamination,…) and disinfection (use of soap or alcoholic hydrogel, air cleaning devices,…).

First, we have considered the interaction of materials with the virus. Since this interaction is mediated by the spike S glycoprotein that covers the viral particle, we have considered the interaction of S (protruding from a virion) with surfaces of different materials of interest. We have considered common materials such as cellulose, graphite and polystyrene. We found that graphite substantially deforms the S protein [1]. On the contrary, the S protein adsorbs over cellulose with little deformation, by forming hydrogen bonds between its receptor binding domain and adjacent residues and the cellulose (some of them mediated by hydration) [1]. In the case of polystyrene, we found strong interaction of S with that material either with the receptor binding domain of S or the sugars (glycans) covering S, depending on the S conformation (open or closed state) [3]. Ongoing investigations of the interaction of S with metals (as included in virucidal materials in the form of nanoparticles for example) are under way. We have also studied the interaction with human skin. We found a substantial difference depending on whether the skin is covered or not by sebum. S protein has little interaction with the sebum covering certain regions of the skin but it is able to adsorb by hydrogen bonds with lipids exposed in the skin in absence of sebum.

Concerning the interaction with chemicals [3], MD simulations of a coarse-grain model of the virus and surfactants show that the disinfection action of soap may occur mostly by blocking the S protein instead of disrupting the envelope membrane. Atomistic MD simulations of the envelope in contact with ROS species show that OH* radicals are able to penetrate into the hydrophobic region of the envelope mainly in protein-lipid contacts, thus being able to disrupt the viral envelope by oxidation and suggesting an effective method for ambient disinfection.

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References

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