Computer simulations of the effect of surfactants to the SARS-CoV-2 virion

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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 Soft Matter, this virus is made by a vesicle-like envelope of proteins and lipids of 90 nm of diameter which tightly encapsulate 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 two main research line. The first line was to develop atomistic molecular dynamics simulations of the interaction of the virus with materials such as cellulose, graphite, polystyrene or the human skin [1-3] in order to provide physico-chemical basis for questions such as the design of better protective equipment or the possible role of indirect virus transmission. After our success in the study of virus-materials interaction, we have considered the question of the interaction of the virus with common disinfection chemical agents such as surfactants. In spite of the importance of the use of soap as a virucidal agent not only in the particular case of SARS-CoV-2, but for enveloped viruses, little is known about the molecular details of the action of surfactants over an enveloped virus. Questions such as the possible inactivation of the virus (by a coverage or denaturation of the spike protein by surfactants) or the damage of the virus integrity (by opening of a pore or hole at the lipid-protein envelop structure) or even the possibility of virus envelope dissolution are discussed here by Molecular Dynamics simulations. For a general exploration of the relative importance of surfactant characteristics and the relative importance of different interactions (surfactant-lipid envelope or surfactant-protein envelope) we have considered coarse-grain (CG) model of a full virus a CG models of surfactants. For a more detailed exploration in the case of common surfactants, we have considered all-atomic MD simulations of representative patches of the virus envelope (containing a mixture of lipids and membrane M proteins at realistic compositions with and without inserted S protein) in contact with common anionic and cationic surfactants such as SDS and CTAB.

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FIGURES

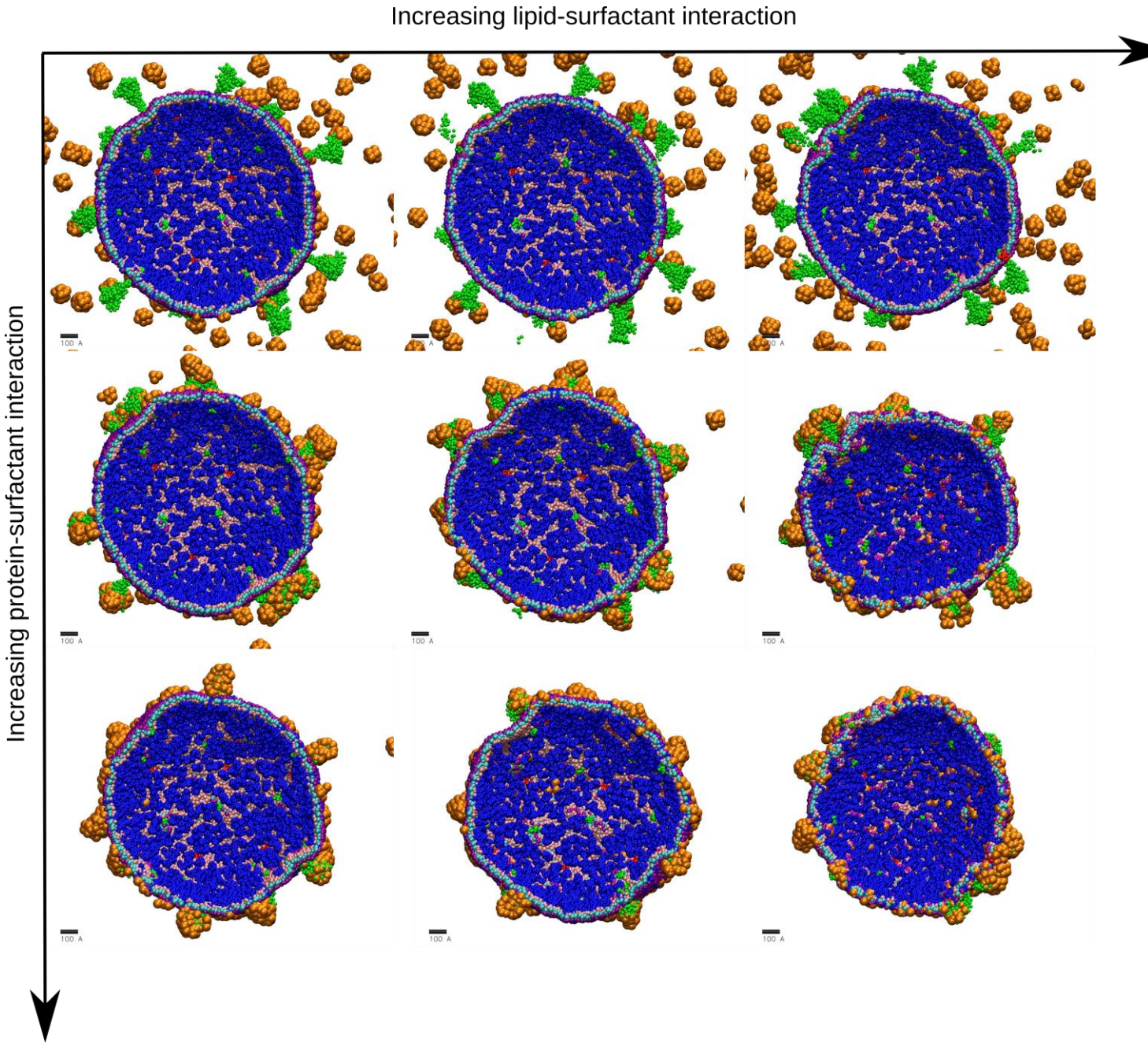

Figure 1: Simulation snapshots showing the effect of surfactant on the structure of a virion particle from CG molecular dynamics simulations for different strengths of the relevant interactions between the surfactants and the virion components. The surfactants are shown in orange, the Spike, M and E virus structural proteins are shown in yellow, blue and red respectively and the different beads of the phospholipids of the envelope are shown in cyan and pink. The scale bar corresponds to 10 nm.