

Interaction between SARS-CoV-2 virus and human skin

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The novel coronavirus SARS-CoV-2 emerged in December 2019 as a human pathogen[1] that caused the COVID-19 disease world pandemic. Therefore, it is clear that emerging infectious diseases caused by coronaviruses must be seen as a major threat to human health.

The transmission of respiratory viruses in general (including coronaviruses and SARS-CoV-2 in particular) involves the expiratory emission of virus-containing aerosols and droplets[2] which may infect other individuals via direct or indirect mechanisms. The direct mechanism involves inhalation of aerosols or the deposition of emitted droplets on mucosal surfaces (e.g. mouth, eyes). Indirect transmission may occur through physical contact with virus containing aerosols and droplets deposited onto materials (exposed surfaces of common objects such as furniture or electronic gadgets, textiles, protective equipment,) and by itself inoculation of virus into the mouth.

The possibility of contamination of human skin by infectious virions plays an important role in indirect transmission of respiratory viruses but little is known about the fundamental physico-chemical aspects of the virus-skin interactions. In the case of coronaviruses, the interaction with surfaces (including the skin surface) is mediated by their large glycoprotein spikes that protrude from (and cover) the viral envelope.

We perform all atomic simulations between the SARS-CoV-2 spike glycoprotein and human skin models[3]. We consider an oily skin covered by sebum and a clean skin exposing the stratum corneum as seen in Figure 1. The simulations show that the spike tries to maximize the contacts with stratum corneum lipids, particularly ceramides, with substantial hydrogen bonding. In the case of oily skin, the spike is able to retain its structure, orientation and hydration over sebum with little interaction with sebum components. Comparison of these results with our previous simulations of the interaction of SARS-CoV-2 spike with hydrophilic and hydrophobic solid surfaces[4], suggests that the soft or hard nature of the surface plays an essential role in the interaction of the spike protein with materials.

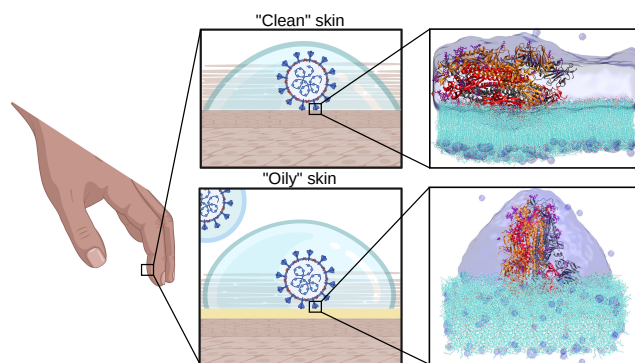


Fig. 1. Scheme of the interaction between SARS-CoV-2 spike glycoprotein and human skin models. The "oily" skin model is covered by sebum and the "clean" skin model exposes the outermost layer of the skin (Stratum Corneum). Reprinted from M. Domingo and J. Faraudo, *Soft Matter*, **17**, 9457 (2021). Licenced under CC BY-NC 3.0 [5].

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