



سمینار هفتگی ماده چگال نرم

Conformational transition of SARS-CoV-2 RBD protein from the down state to the up state

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Abstract

Since the first recorded case in December 2019, over 60 million people have been infected by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Among the structural parts of this virus, the trimeric spike glycoprotein, located on the viral membrane, plays a pivotal role, as it is responsible for virus attachment and entry to the host cells. The spike glycoprotein undergoes hinge-like conformational movements and its receptor-binding domains (RBD) can be in either an accessible (up) state or an inaccessible (down) state to the host cell receptors. Therefore, by simulating the conformational transition of RBD from its down state to the up state, it is possible to investigate the important properties of this transition and recognize the key amino acids for further studies such as the effects of amino acids' modification on this transition.

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