

SUPPLEMENTARY INFORMATION

Modeling the Interaction of SARS-CoV-2 Binding to the ACE2 Receptor by Molecular Theory of Solvation

Alexander E. Kobryn^{1,*}, Yutaka Maruyama², Carlos A. Velázquez Martínez³, Norio Yoshida⁴,
Sergey Gusarov^{1,*}

¹Nanotechnology Research Centre, National Research Council Canada, 11421 Saskatchewan Drive NW, Edmonton, Alberta, T6G 2M9, Canada

²Architecture Development Team, FLAGSHIP 2020 Project, RIKEN Center for Computational Science, Kobe, Hyogo 650-0047, Japan

³2142-L Katz Group Centre for Research, University of Alberta, 11315-87 Avenue NW, Edmonton, Alberta, T6G 2H5, Canada

⁴Department of Chemistry, Graduate School of Science, Kyushu University, 744, Motooka, Nishi-ku, Fukuoka, 819-0395, Japan

* Corresponding authors; Emails: alex.kobryn@nrc-cnrc.gc.ca, sergey.gusarov@nrc-cnrc.gc.ca

CONTENTS

Multimedia: video_(0A).webm

Multimedia: video_(4A).webm

DESCRIPTION

Both videos show the geometry when ACE2 receptor and SARS-CoV-2 spike proteins come to a close contact. The file “video_(0A)” refers to the initial geometry while the file “video_(4A)” refers to the case when separation between proteins increases for additional 4 Å. The initial geometry is taken from the Protein Data Bank as described in the main text. Proteins are sketched as rainbow colored solid ribbons.

At first, the ACE2 receptor is on the left and painted in brighter colors while the SARS-CoV-2 spike is on the right and is painted in darker colors. The whole structure rotates for 180 degrees with respect to a vertical axis.

After the first rotation, the display of the first solvation shell formed by the water oxygen is turned on. The shell is painted in red, the inner part of the isosurface, if exposed, appears in gray. To ensure that the first solvation shell is seen all around the proteins the selected isosurface numerical value is relatively low: 1.5. The whole structure rotates for another 180 degrees, proteins are not seen as they are completely inside the solvation shell.

Next, to let one see inside the solvation shell, a clipping plane is turned on. It cuts (makes invisible) the front part of the shell and allows proteins sketches to be viewable, the remaining part of the shell appears behind the sketches. The whole structure rotates for another 180 degrees, at the end of rotation the proteins are not seen again as the visible part of the solvation shell comes to the front view. This ends the movies.

The purpose of video demonstrations described above is to help readers in understanding the 3D-RISM approach, in particular, how the computation results are visualized. Typically, a visual examination is the first one, however it affect the consecutive analysis and the conclusion of the whole study.