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# Computational Insights into the Allosteric Effect and Dynamic Structural Features of the SARS-COV-2 Spike Protein


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**Invited for the cover of this issue are Aiqian Zhang, Jianjie Fu, Guibin Jiang, and co-workers at the Chinese Academy of Sciences. The image depicts the molecular recognition of human angiotensin-converting enzyme 2 by the SARS-COV-2 spike protein. Read the full text of the article at 10.1002/chem.202104215.**

### *What is the most significant result of this study?*

We have successfully revealed the allosteric effect of the SARS-COV-2 spike protein binding with ACE2. The intermolecular interaction can cause a centripetal movement of the receptor-binding domain of the spike protein with a change in the dihedrals of key residues such as F329 and F515. An allosteric communication pathway Q493-L452-L492-R454-N422-Y423-V512 has been identified for the conformation transition from the "up" state to the "ACE2-bound 1" state, which is accompanied by the exposure of two potential cleavage sites to the surface. Moreover, in comparison with that of SARS-COV, the higher affinity of SARS-COV-2 with ACE2 can be partially ascribed to the replacements V404→K417 and D480→S494 in the spike protein.

### *Is your current research mainly curiosity driven (fundamental) or rather applied?*

The ever-increasing number of new chemicals and diverse toxicological endpoints make it both impractical and infeasible to accomplish the goal of risk assessment and management by solely depending on experimental analysis. Our current research focuses on the molecular mechanism of toxicology and environmental behavior for selected pollutants through data-driven learning and theoretical simulation with necessary experimental verification, which in turn provides efficient computational tools for tackling environmental issues.

### *What other topics are you working on at the moment?*

In addition to the work on molecular recognition mechanism of SARS-COV-2, we are also active in the related research topics at the moment; chemical-SARS-COV-2 interaction, and altered chemical exposure pattern such as enhanced hand-to-mouth exposure from hand sanitizers during the COVID-19 pandemic.