# Multiscale Modeling of Binding SARS-CoV-2 to Various Substrates

The Stony Brook Multiscale Model Team

April 8, 2020

**PI:** Peng Zhang, Applied Mathematics and Statistics

**Co-PIs:** Yuefan Deng, Applied Mathematics and Statistics

Miriam Rafailovich, Materials Science and Chemical Engineering

Marcia Simon, Oral Biology and Pathology, Dermatology, School of Medicine

## Project Summary

**Background**: The SARS-CoV-2 has infected, globally, more than 1.5M people of which the US accounts for more than 28%, only 2-3 months after its outbreak. Its conformation and binding sites are understood while its other properties including infection intensity and stability on various substrates such as copper, cupboard, plastic, and stainless steel, as well as human tissues are still elusive. To understand the infection, we start from analyzing the binding on these substrates under such external conditions as temperature and pH values, by orchestrated efforts in vitro and in silico experiments. **Innovation**: our multiscale model uses the learned parameters with big data collected through these experiments with the key thrust in accelerating the conventional all-atomic MD by 5~6 orders of magnitude, leveraging on our decade-long study of a similar model of platelet aggregation and adhesion to human blood vessels. Our study will provide guidelines for development of preventive strategies including personal protective equipment of various kinds. Of course, the entire model can be generalized conveniently to study other virus on a variety of surfaces.