



**ACS** Local Section  
New York  
Computers in Chemistry

# FROM CLOSED TO OPEN: OMICRON MUTATIONS INCREASE INTERDOMAIN INTERACTIONS AND REDUCE EPITOPE EXPOSURE

**Speaker: Dr. Phu Tang**

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**Date: Friday, April 28, 2023**

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**Time: 11:00 AM EDT via Zoom**



## Abstract

Omicron BA.1 is a highly infectious variant of SARS-CoV-2 that carries more than thirty mutations on the spike protein compared to the Wuhan wild type (WT). Some of the Omicron mutations, located on the receptor binding domain (RBD), are exposed to the surrounding solvent and are known to help evade immunity. However, the impact of buried mutations on the RBD conformations and on the mechanics of the spike openings is evident. We use all-atom molecular dynamics (MD) simulations with metadynamics to characterize the thermodynamic RBD-opening ensemble, identifying significant differences between WT and Omicron. Specifically, the Omicron mutations S371L, S373P, and S375F make more RBD interdomain contacts during the spike's opening. Moreover, Omicron takes longer to reach the transition state than WT. It stabilizes up-state conformations with fewer RBD epitopes exposed to the solvent, potentially favoring immune or antibody evasion.

## Biography

Dr. Phu Tang joined the Center for Computational Mathematics in September 2021 as a Flatiron Research Fellow. Tang's background is in molecular dynamics simulations concentrated on rare events using enhanced sampling methods on collective variables. Tang's other interests include history and digital arts. Tang has a Ph.D. and B.S. in Biochemistry from the City University of New York-College of Staten Island.

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