

**The Hong Kong Polytechnic University  
Department of Applied Mathematics****Seminar****Implicit-Solvent Modeling of Dry-Wet Transitions for Hydrophobic Binding/Unbinding****By****Dr. Shenggao ZHOU  
Shanghai Jiao Tong University****Abstract**

Solvent fluctuations play a fundamental role in many water-mediated biological processes of importance. Capillary evaporation and condensation, induced by solvent fluctuations, take place in hydrophobic confinements. Based on a variational implicit solvent model, we develop the level-set method and the string method to predict dry-wet transitions. The predicted potential of mean force and transition rates for multiple solvation states are further used in newly proposed multi-state Brownian dynamics simulations and related Fokker–Planck calculations for a ligand–receptor system. We find the hydration transitions to significantly slow down the binding process, but significantly accelerate the unbinding process. Moreover, our approach allows the characterization of nonequilibrium hydration states of pocket and ligand during the ligand movement, for which memory and hysteresis present in binding/unbinding processes. Our study thus provides a significant step forward toward efficient, physics-based interpretation and predictions of the complex kinetics in realistic ligand–receptor systems. This is a joint work with Dr. R. G. Weiß, L. Cheng, J. Dzubiella, J. A. McCammon, and B. Li.

[Click to join \(Zoom\)](#)**Date: 16 February 2022 (Wednesday)****Time: 10:00-11:00 (Hong Kong Standard Time GMT +8)****Venue: Online Talk via Zoom (Meeting ID: 929 3839 4099)****Speaker: Dr. Shenggao Zhou, Shanghai Jiao Tong University****Host: Prof. Zhonghua Qiao, The Hong Kong Polytechnic University****Click to join:****<https://polyu.zoom.us/j/92938394099?pwd=YUF0Yi9DT3JzamJmdVRXTks5dDZJQT09>****\* \* \* ALL ARE WELCOME \* \* \***For enrolment, please send your name and email to [wai-yan.moon@polyu.edu.hk](mailto:wai-yan.moon@polyu.edu.hk) on or before 15 February 2022