

**SAMPLING FOR DYNAMIC-STRING ENZYME REACTION SIMULATIONS: AN IMPROVE ON-THE-PATH RANDOM WALK METHOD** Wei Yang, Department of Chemistry and Biochemistry, Florida State University, Institute of Molecular Biophysics, Tallahassee, FL 32306.

The on-the-path random walk sampling algorithm enables the first generalized ensemble based dynamic string reaction path calculations. In this talk, the further development and application on multi-step and multi-coordinate enzyme reactions will be presented.