

MAR05-2004-001960

Abstract for an Invited Paper  
for the MAR05 Meeting of  
the American Physical Society

### **Single-Molecule Studies of Enzymatic Structure-Function Dynamics**

HAW YANG, Department of Chemistry, UC Berkeley, and Physical Biosciences Division, LBNL, Berkeley, CA 94720

Many biological macromolecules rely on some form of conformational flexibility to perform their designated tasks. This flexibility can be a factor in such important effects as cooperativity and allostery, or in providing the basis for entropic control. The structural origins and functional manifestations of enzymatic flexibility, however, are still poorly understood. Förster Resonance Energy Transfer (FRET) mediated measurements of intra-molecular distance in single molecules can help to bridge this gap. In this way, the 3D structural motions of individual AKe molecules were projected on the 1D coordinate,  $q$ , defined by the placement of FRET probes. Here, we report the application of single-molecule time-resolved FRET to measuring the conformational fluctuation of adenylate kinase from *E. coli* (AKe) under reactive conditions. The velocity-position time traces on the  $(\dot{q}, q)$  configuration space were acquired from single AKe molecules. Information about reaction dynamics was extracted photon-by-photon using the recently developed maximum-information and change-point methods. The structure-function dynamics will be discussed from the perspective of such configuration-space trajectories.