Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Linking enzyme conformational dynamics to catalytic function with single-molecule FRET YAN-WEN TAN, JEFFREY A. HANSON, Dept of Chemistry, UC Berkeley, KARL DUDERSTADT, Biophysics Graduate Group, UC Berkeley, SUCHARITA BHATTACHARYYA, Dept of Chemistry, UC Berkeley, HAW YANG, Dept of Chemistry, Biophysics, UC Berkeley & Physical Biosciences Division, LBNL — Many enzymes endure sizable conformational remodeling on a timescale comparable to their catalytic cycle. These conformational dynamics may be critical to the enzymes' catalytic function. In adenylate kinase (AK) from *E. coli*, this involves a large-amplitude rearrangement of the enzyme's lid domain. We use high-resolution single-molecule FRET developed in our laboratory to measure AK's domain movements on its catalytic timescale. We utilize maximum entropy-based methods to remove photon-counting noise from raw data, so that the enzyme's entire conformational distribution can be quantitatively recovered without a presumed model. Multiple sequence alignment suggests regularities between the conserved residues and their structural-functional roles. Armed with precise single-molecule FRET dynamics measurements and comprehensive bulk kinetic studies of the mechanism, we were able to quantitatively correlate AK's stochastic lid dynamics with its deterministic catalytic rates. Implications on the structure-function conservation and protein engineering will be discussed.

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Date submitted: 04 Dec 2007 Electronic form version 1.4