

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Dynamic Coupling among Protein Binding, Sliding, and DNA Bending Revealed by Molecular Dynamics CHENG TAN, Kyoto Univ, TSUYOSHI TERAOKAWA, Columbia Univ, SHOJI TAKADA, Kyoto Univ — Protein binding to DNA changes the DNAs structure, and altered DNA structure can in turn modulate the dynamics of protein binding. This mutual dependency is crucial for genome organization, but poorly understood. Here we investigated dynamic couplings among protein binding to DNA, protein sliding on DNA, and DNA bending by applying coarse-grained simulations to the bacterial architectural protein HU and 14 other DNA-binding proteins. First, we showed that the simulated HU exhibits a strong preference for DNA gap, consistent with biochemical experiments. The high anity was attributed to a local DNA bend. The long-time dynamic analysis revealed that HU sliding is associated with the movement of the local DNA bending. Deciphering single sliding steps, we found the coupling between HU sliding and DNA bending is akin to cation transfer on DNA and can be viewed as a protein version of polaron-like sliding. Interestingly, on shorter time scales, HU paused when the DNA was highly bent and escaped from pause once the DNA spontaneously returned to a less bent structure. With 14 other proteins, we explored the generality and versatility of the dynamic coupling and found that 6 assayed proteins exhibit the polaron-like sliding.¹

¹C. Tan *et al.*, *JACS* 2016, 138, 8512.

Cheng Tan
Kyoto Univ

Date submitted: 10 Nov 2016

Electronic form version 1.4