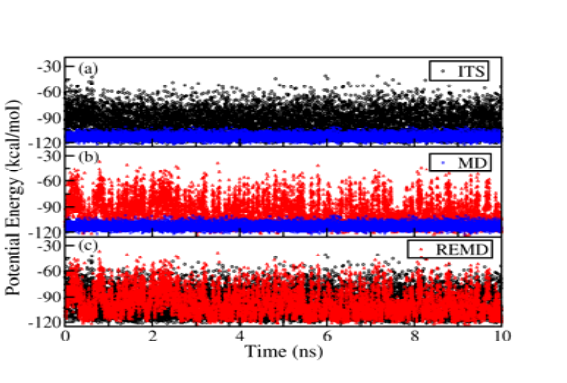
Enhanced Sampling of Protein Conformations

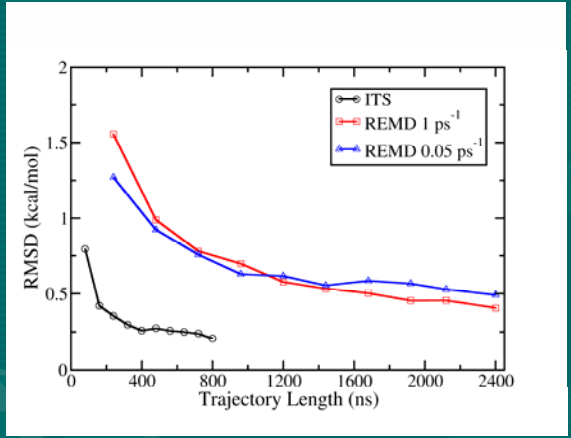
Yi Qin Gao, Department of Chemistry, Texas A&M University, College Station, TX 77843

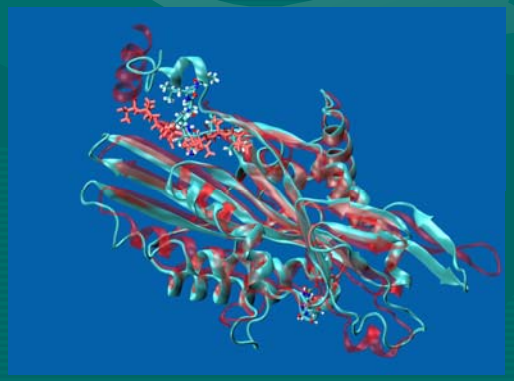
A new and efficient enhanced integrated temperature sampling (ITS) method was developed. This method combines the advantages of replica exchange (REMD) and multicanonical simulation methods and is more efficient in configuration sampling and thermodynamics calculations of large systems.



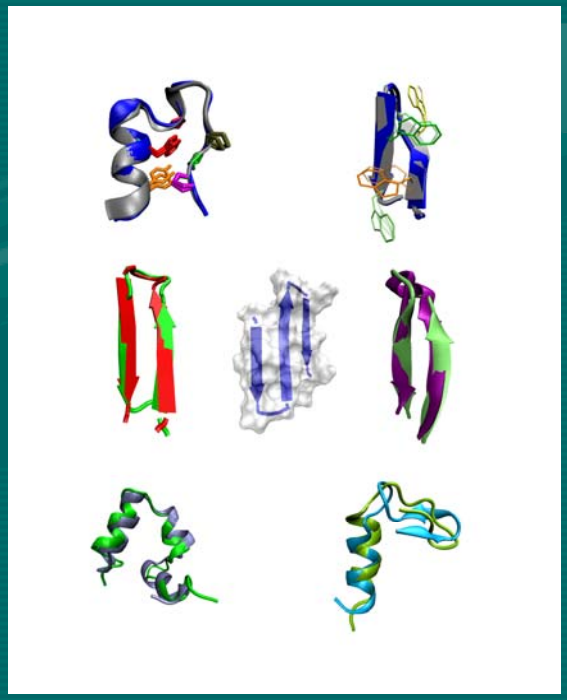
The sampled energy for ala-prol shows that ITS is more efficient in the sampling in the energy space than both normal MD and REMD.

The convergence in thermodynamics calculations is significantly faster for ITS than for REMD.





Enhanced sampling simulations showed that the conformational change of kinesin from the ADP occupied structure (red) to ATP occupied structure (blue).



Examples of proteins folded using the ITS calculations. Application of ITS allows fast calculation of protein folding thermodynamics.