Students' Annual Seminar

Collective Variable Optimization for Bio-molecular Systems

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Quantifying any bio-molecular recognition process depends on the chosen collective variables (CVs). Sometimes it is misleading to put same weights on all the CVs. In many cases these involves unequal weights for the CVs chosen. Dimensional reduction technique will give us valuable information regarding the contribution of each CVs along each of the reduced dimensions. Here we have performed different dimensional reduction techniques taking a simple system. Our system is the popular prototypical cavity-ligand in explicit water. Here these techniques have been used to get the fraction of contribution of the chosen CVs. We have found that water plays a very important role in the unbinding process. In this talk, I will show how crucial role water is playing in the unbinding process.

Friday, Mar 1ˢᵗ 2019

11:45 AM (Tea/Coffee at 11:30 AM)

Seminar Hall, TIFR-H