



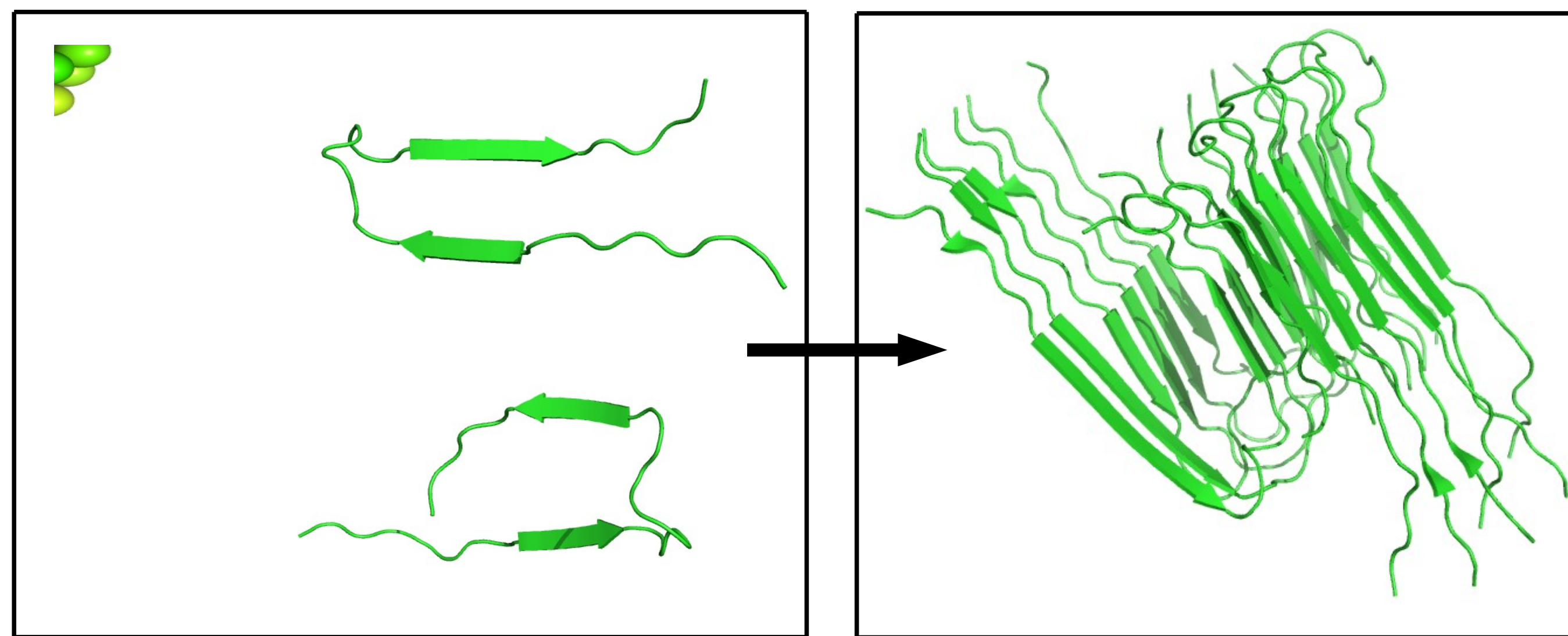
Specific Interactions In A Coarse Grained Hard Sphere Model



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Introduction/Outline

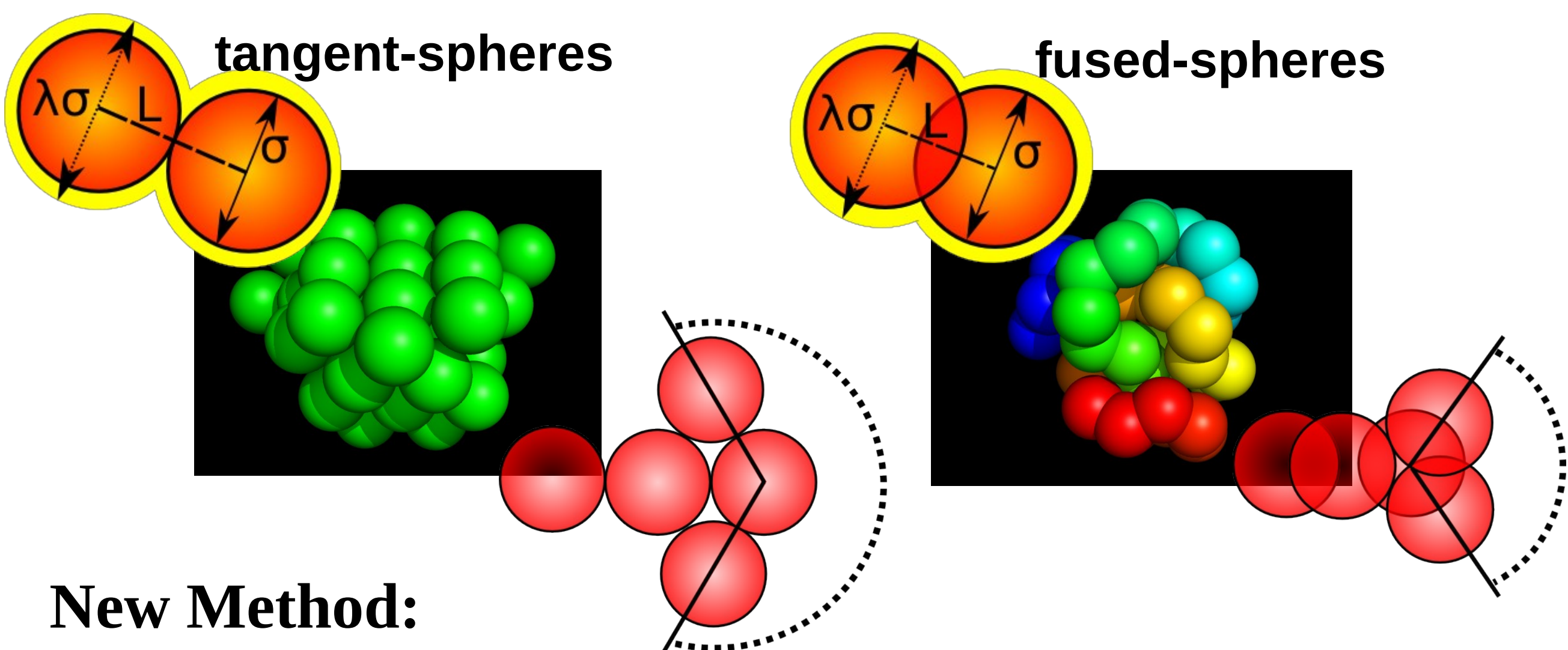
We start by creating a coarse grained model chain with a defined intramolecular structure (e.g. β -structure like).



Model/Method

$$H = \sum_{i=1}^N \sum_{j \neq i, i \pm 1}^N (\epsilon \Theta(\lambda_1 \sigma - r_{ij}) + \epsilon_{ij} \Theta(\lambda_2 \sigma - r_{ij}))$$

- ϵ well depth of monomer monomer interaction
- σ hard core diameter
- $\lambda \sigma$ square well diameter of interaction



New Method:

Stochastic Approximation Monte Carlo

$$S(\mathbf{E}, t+1) = S(\mathbf{E}, t) + \gamma_t (\delta_{E_i E_{new}} - 1/n)$$

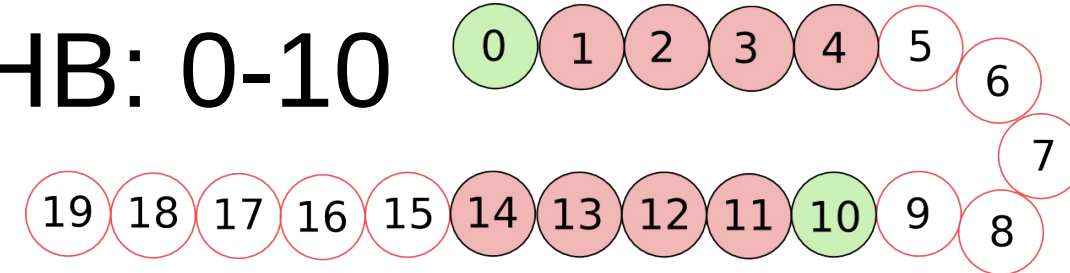
with $\mathbf{E} = (E_1, \dots, E_n)$

plus Umbrella Sampling

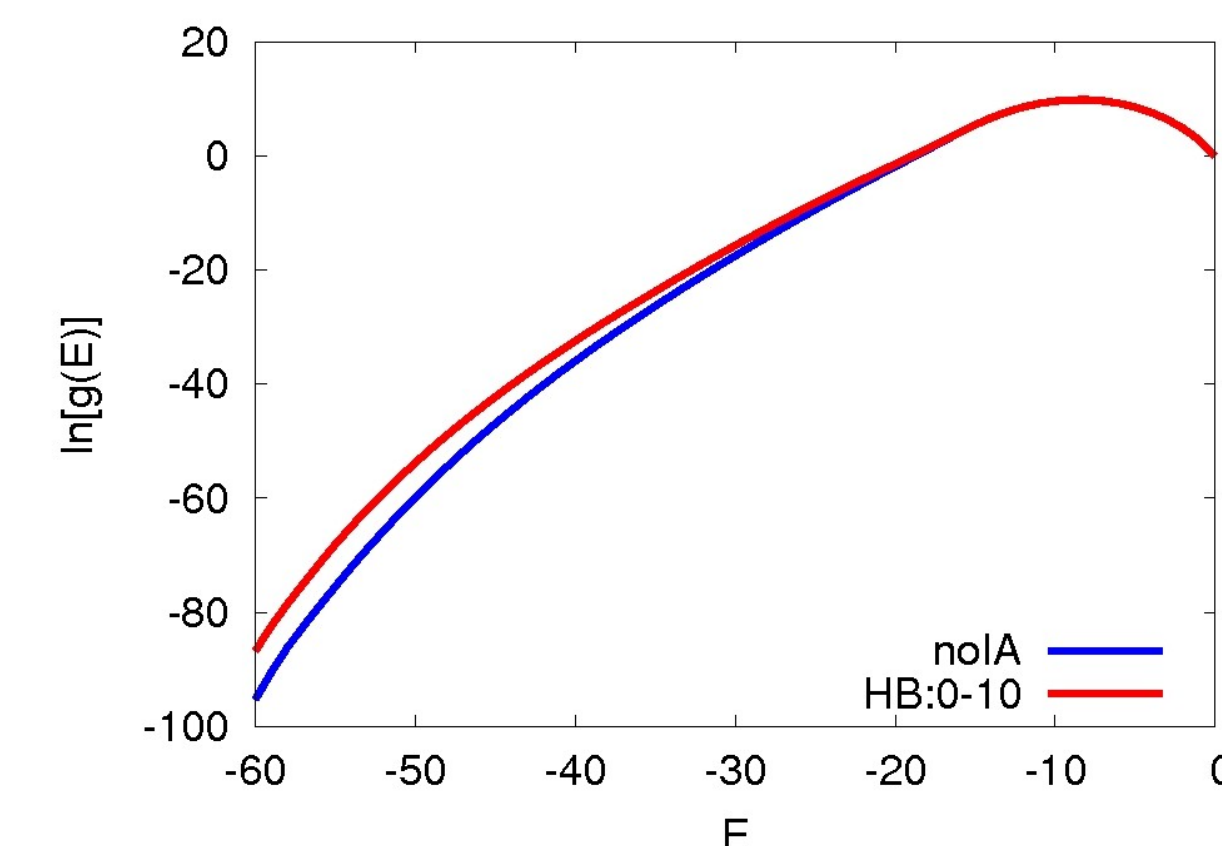
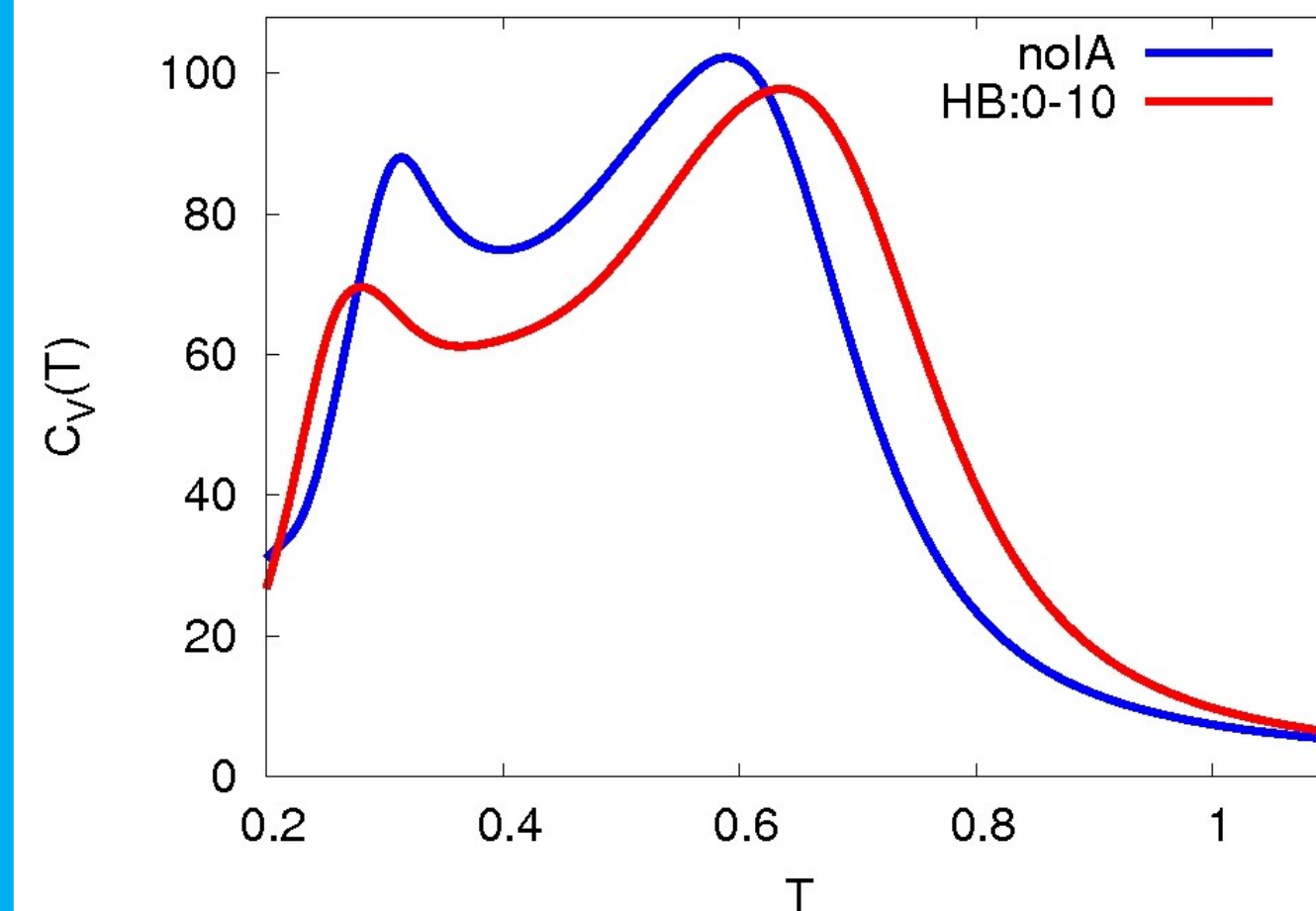
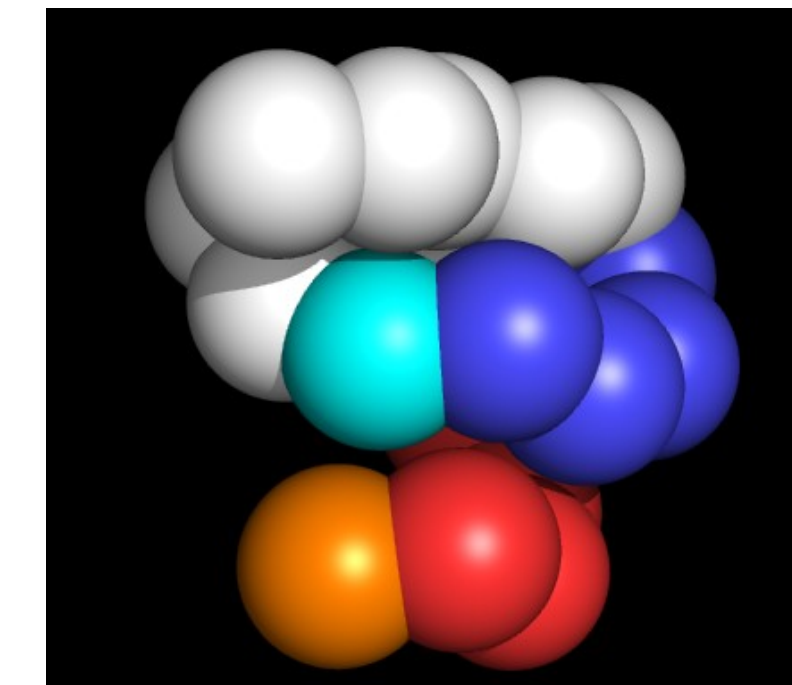
Results

$N=20, \lambda_1 \sigma = 1.1, \lambda_2 \sigma = 1.09, \epsilon = 1, \epsilon_{ij} = 3, L = 0.6$

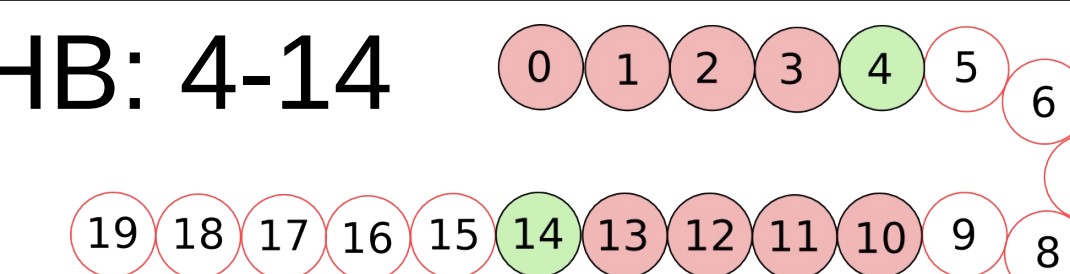
HB: 0-10



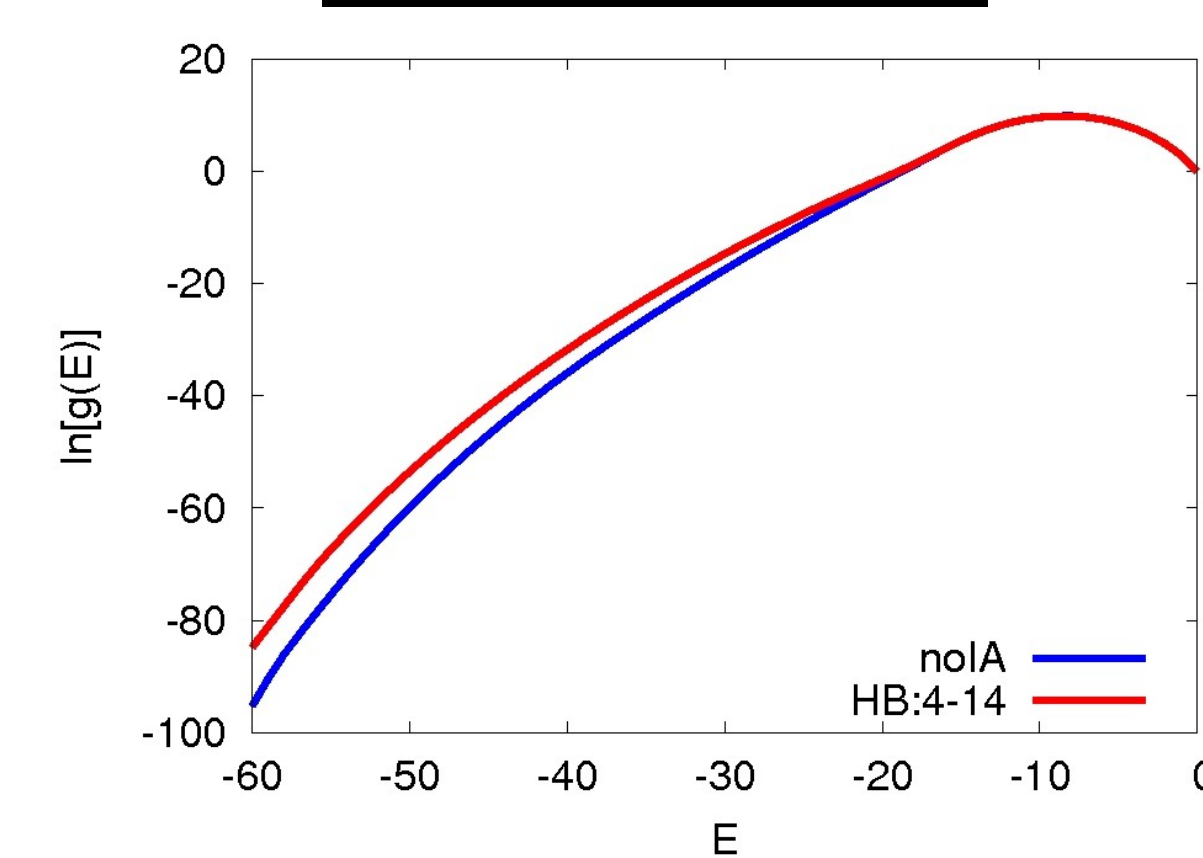
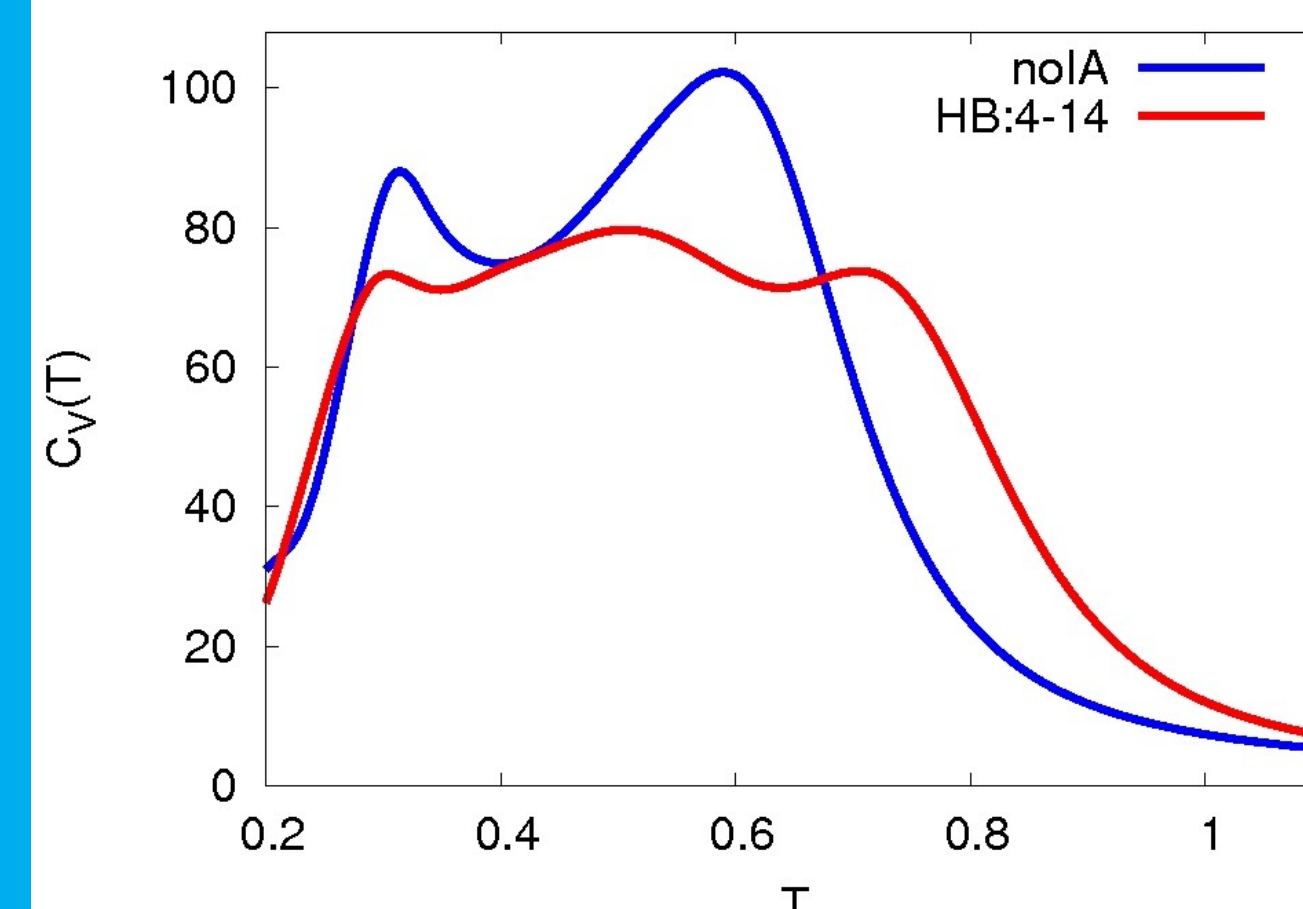
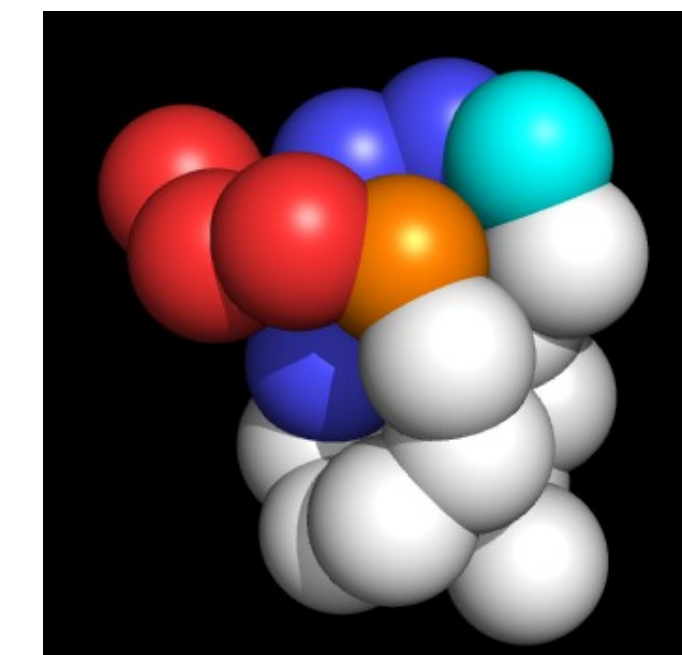
- possible specific interaction
- specific interaction B
- specific interaction A



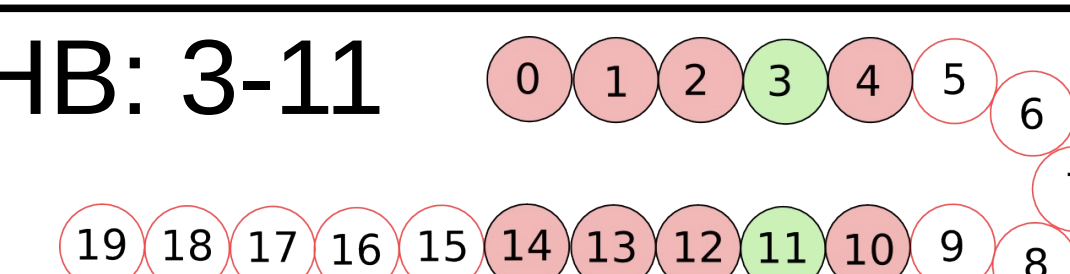
HB: 4-14



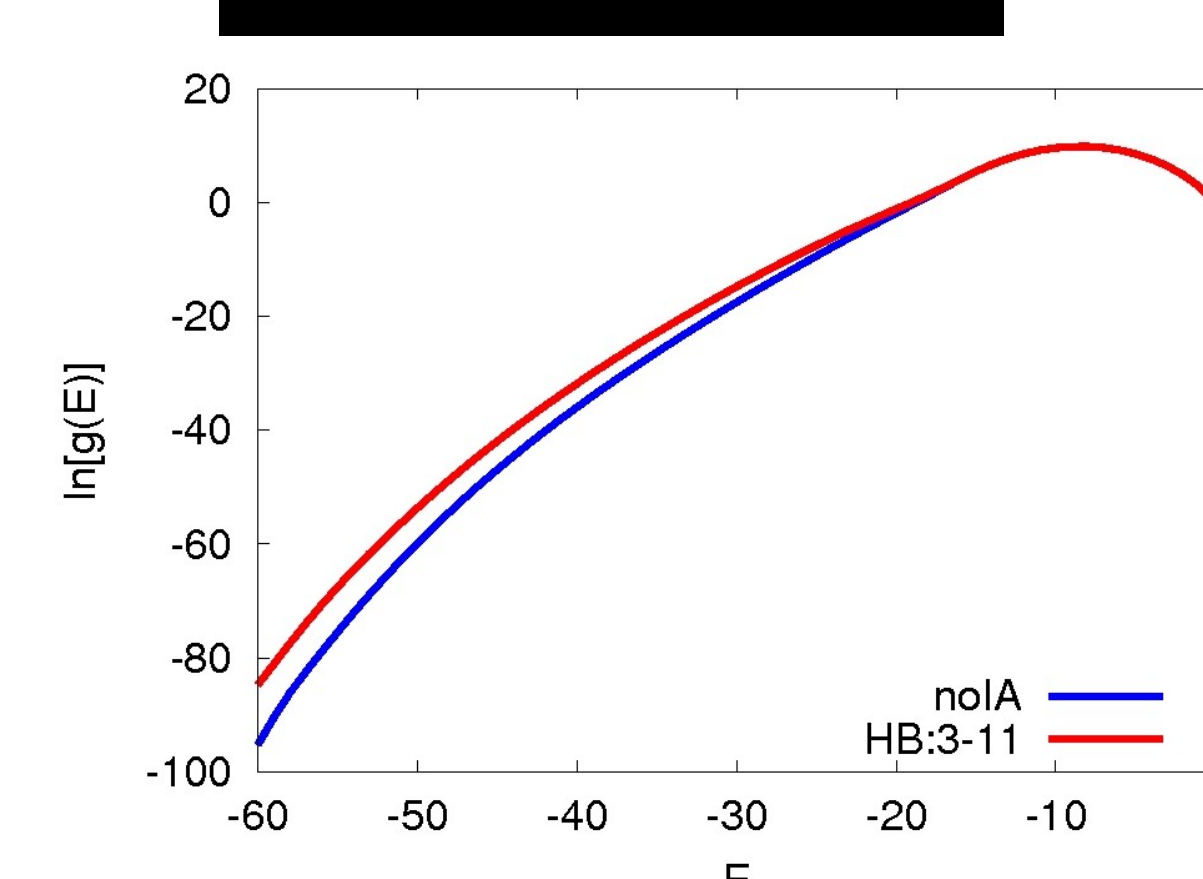
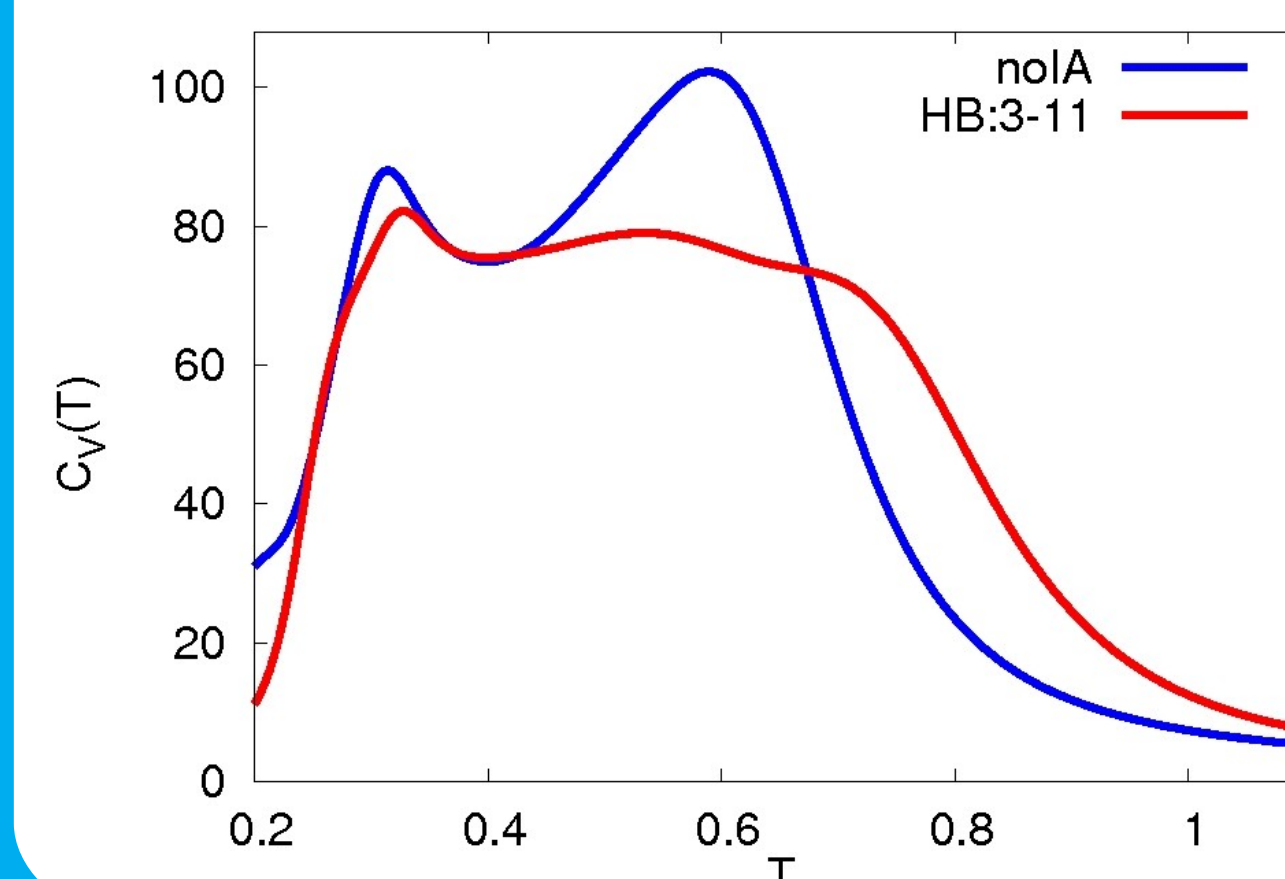
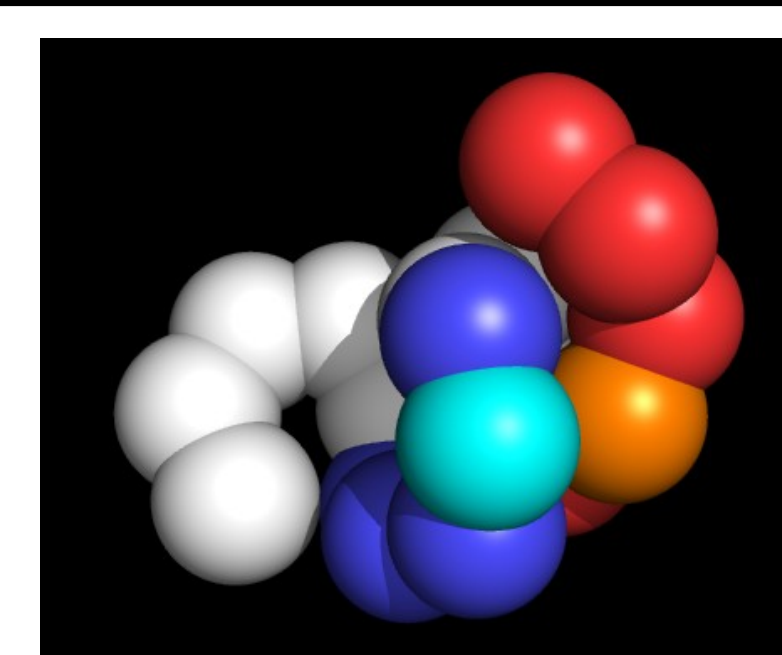
- possible specific interaction
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- specific interaction A



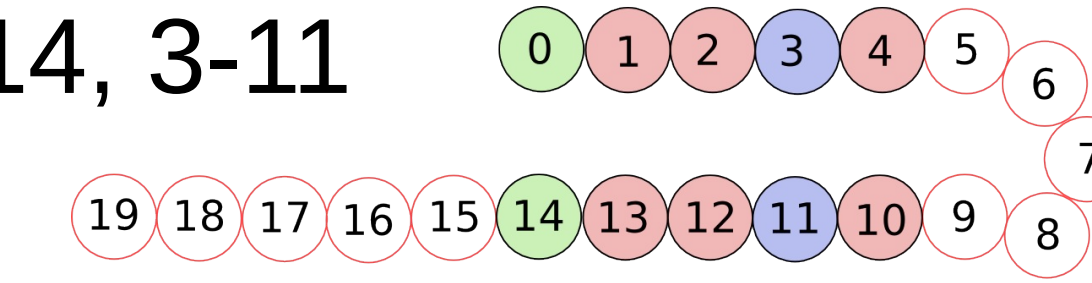
HB: 3-11



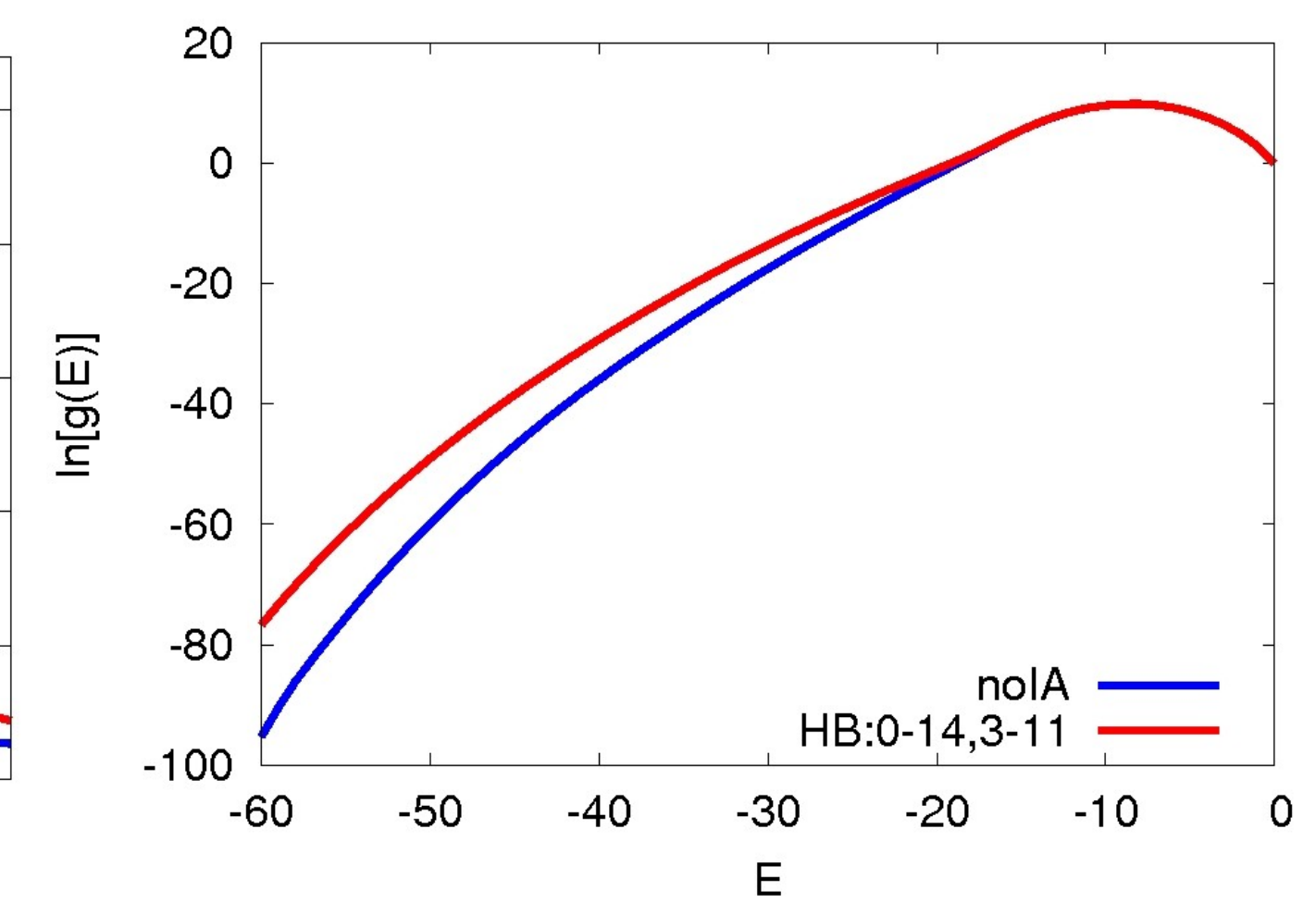
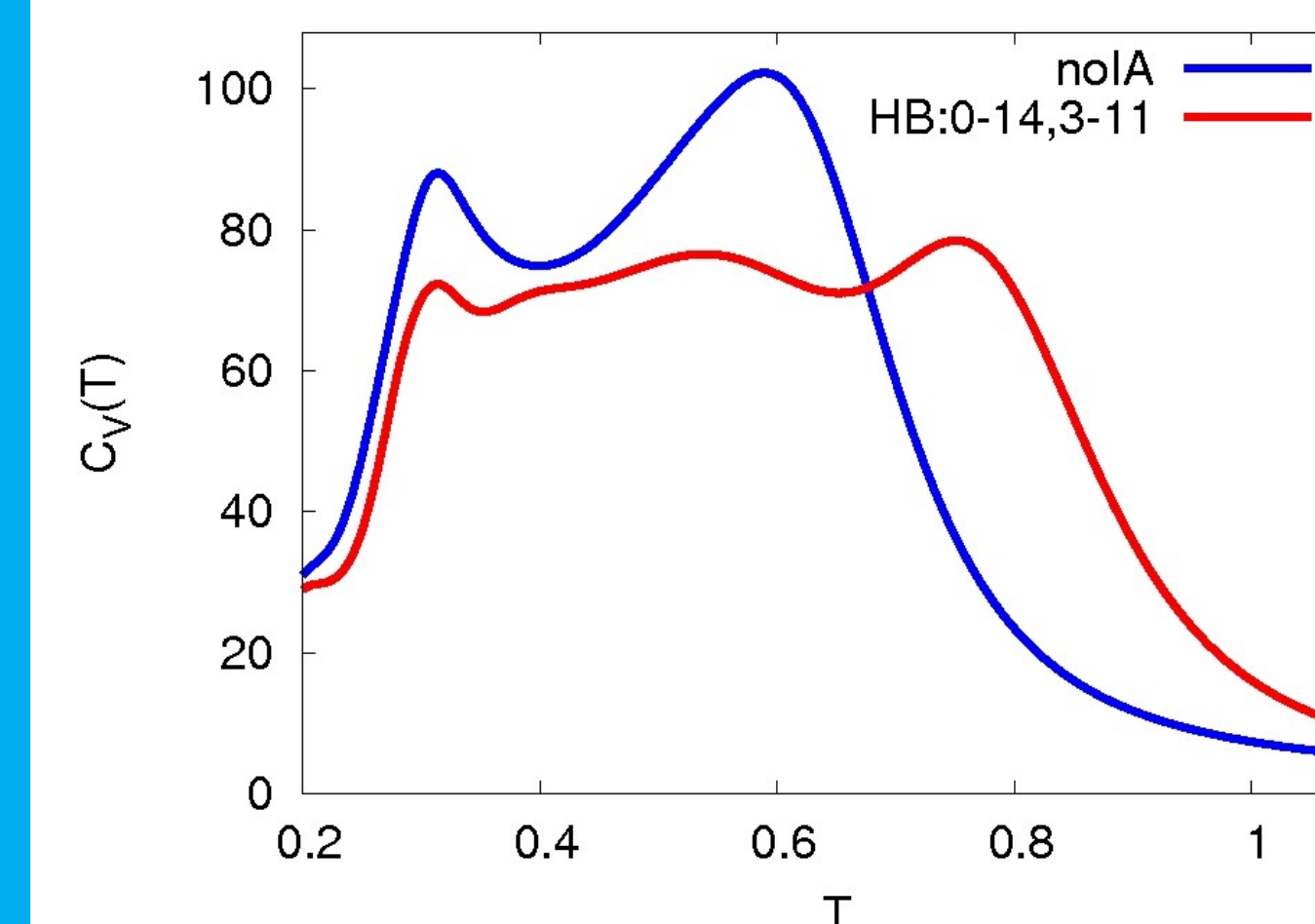
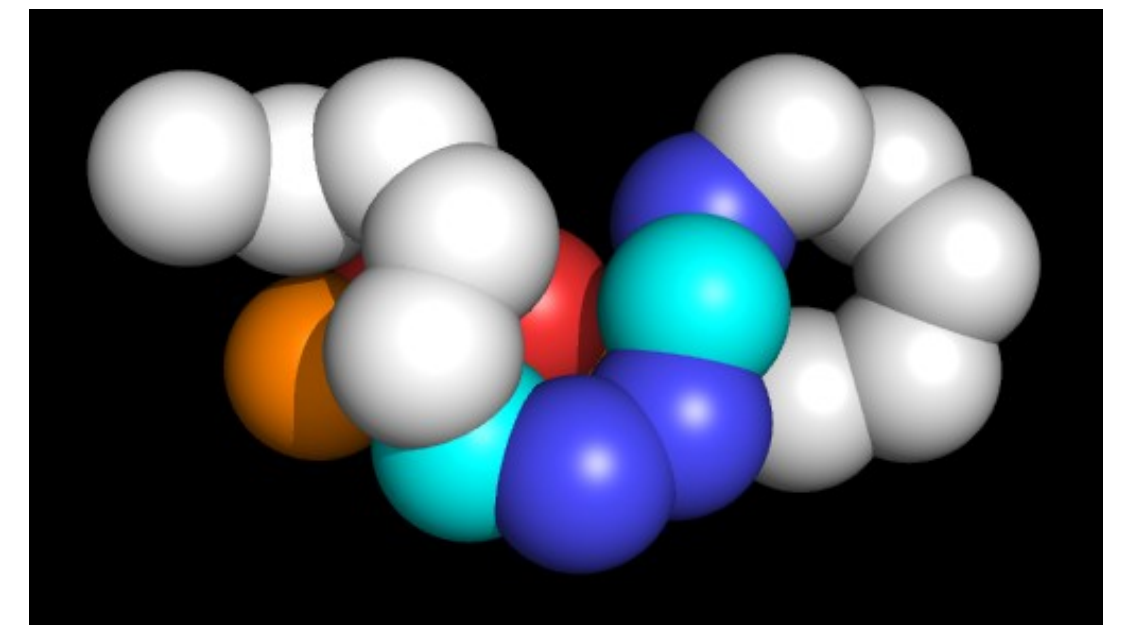
- possible specific interaction
- specific interaction B
- specific interaction A



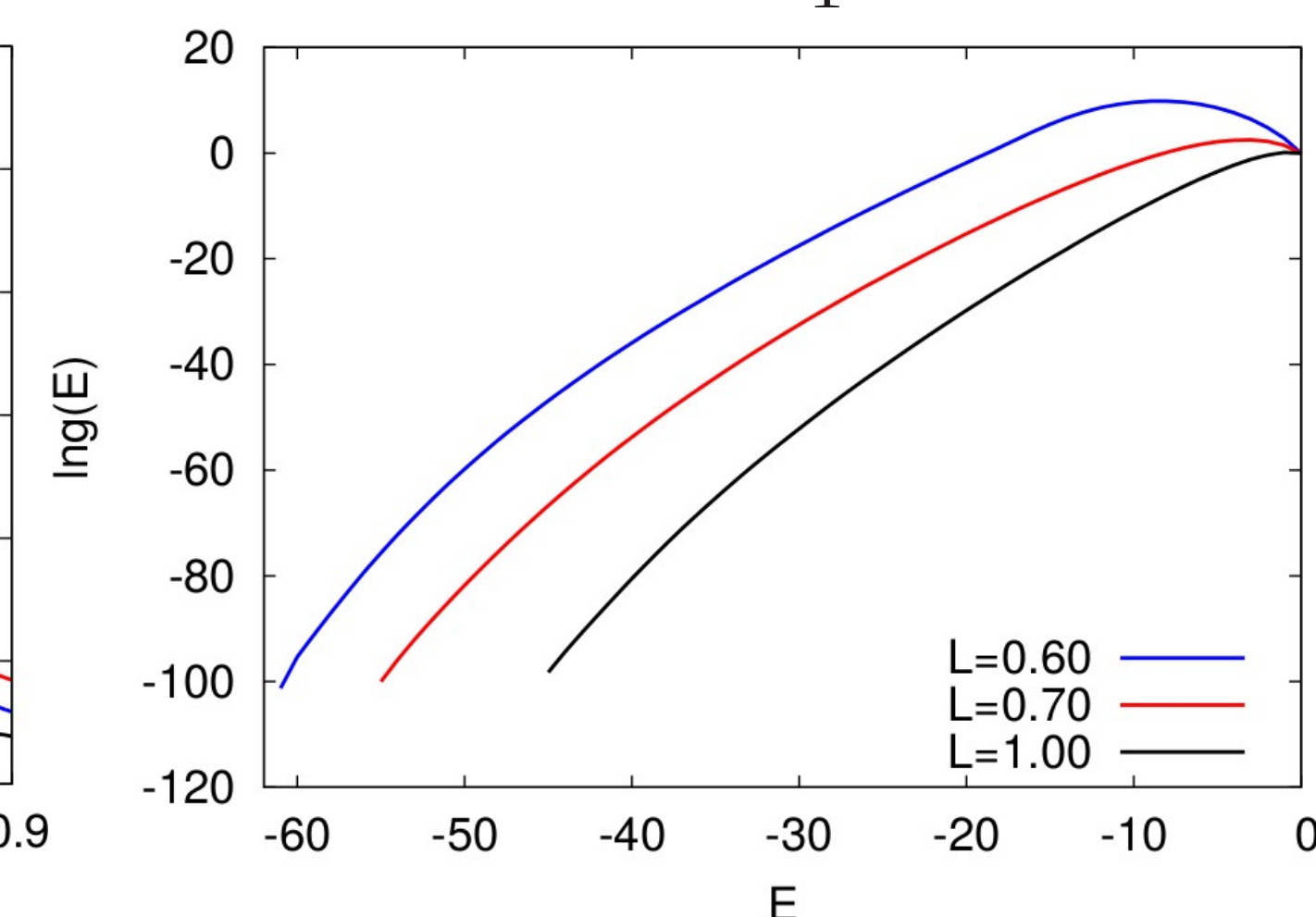
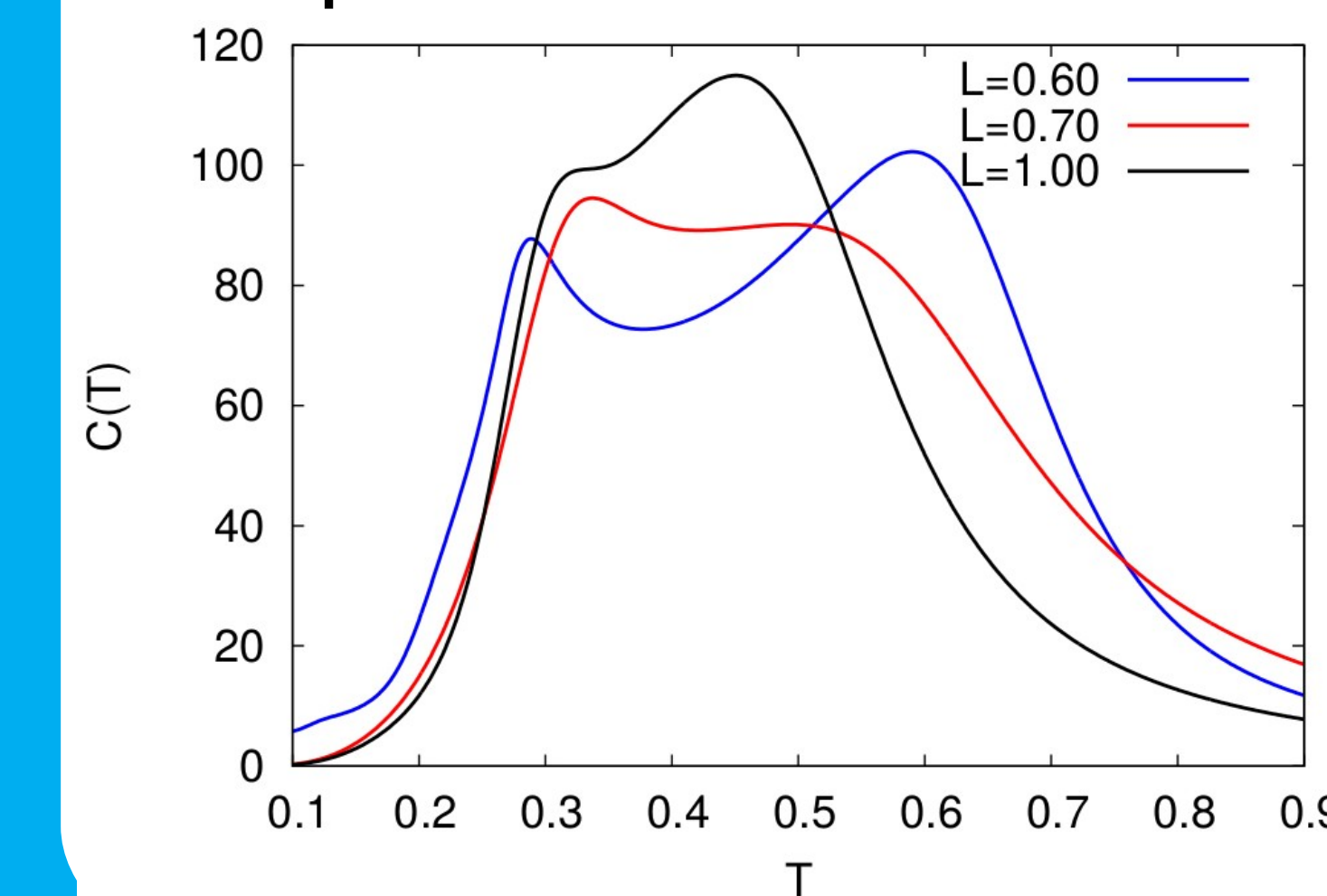
HB: 0-14, 3-11



- possible specific interaction
- specific interaction B
- specific interaction A



Comparison to Non-Interaction chains: $N=20, \lambda_1 \sigma = 1.1$



Outlook

- change from go-like model to donor-acceptor model
- study parameters for donor-acceptor model
- study density dependent aggregation

Literature:

- Mark P. Taylor, Wolfgang Paul, Kurt Binder, Polymer Science, Ser.C, Vol. 55, No.1, pp.23 -38, (2013)
- Faming Liang, Chuanhai Liu, Raymond J. Carroll, J. Am. Statist. Assoc., Vol.102, No.477, (2007)

Project name: Intra- and intermolecular structure formation in the presence of specific interactions