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Multi-scale models for cell adhesion YINGHAO WU, JIAWEN CHEN, ZHONG-RU XIE, Albert Einstein College of Medicine — The interactions of membrane receptors during cell adhesion play pivotal roles in tissue morphogenesis during development. Our lab focuses on developing multi-scale models to decompose the mechanical and chemical complexity in cell adhesion. Recent experimental evidences show that clustering is a generic process for cell adhesive receptors. However, the physical basis of such receptor clustering is not understood. We introduced the effect of molecular flexibility to evaluate the dynamics of receptors. By delivering new theory to quantify the changes of binding free energy in different cellular environments, we revealed that restriction of molecular flexibility upon binding of membrane receptors from apposing cell surfaces (trans) causes large entropy loss, which dramatically increases their lateral interactions (cis). This provides a new molecular mechanism to initialize receptor clustering on the cell-cell interface. By using the subcellular simulations, we further found that clustering is a cooperative process requiring both trans and cis interactions. The detailed binding constants during these processes are calculated and compared with experimental data from our collaborator's lab.

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