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WUHAN TEXTILE UNIVERSITY

The Van der Waals and Electrostatic Interaction Studying of Crystalline Cellulose Iβ Based on Molecular Dynamics

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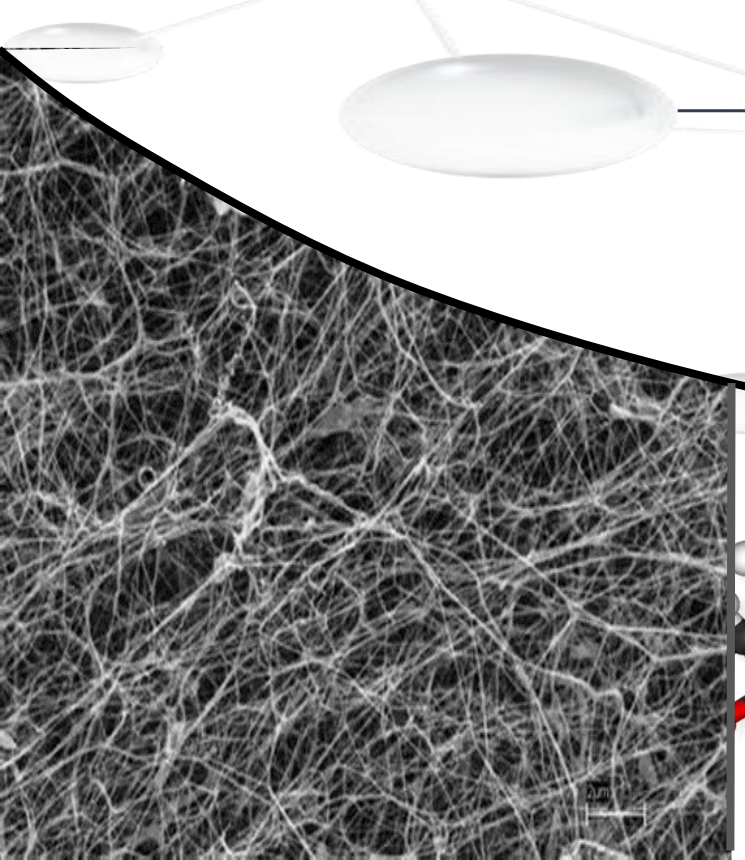
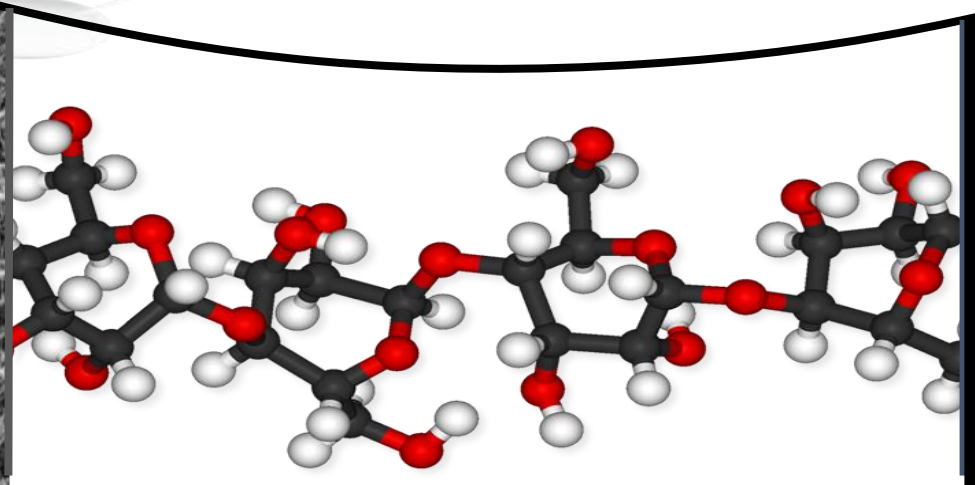
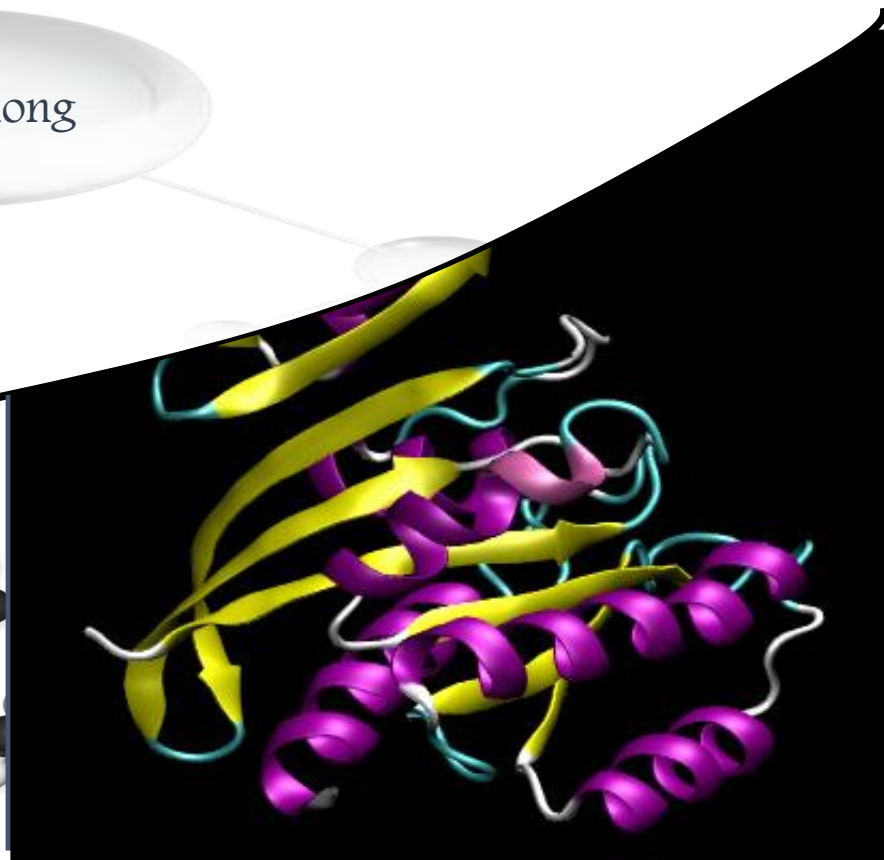
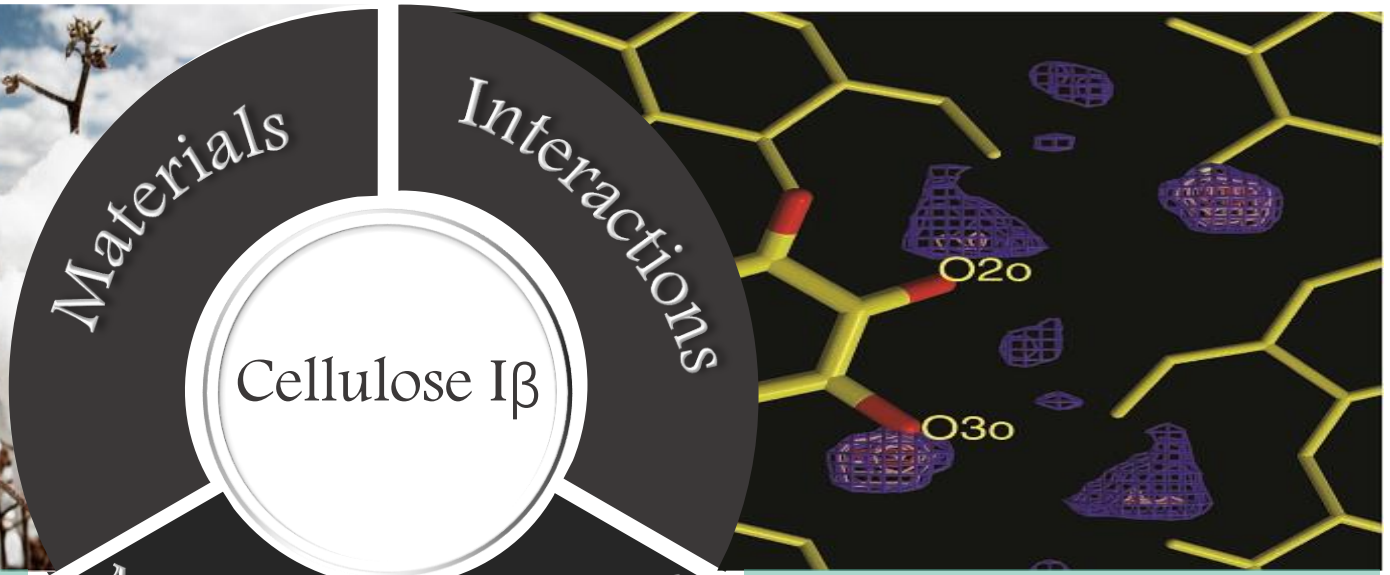






Cellulose fibers are important mature of textile and other materials

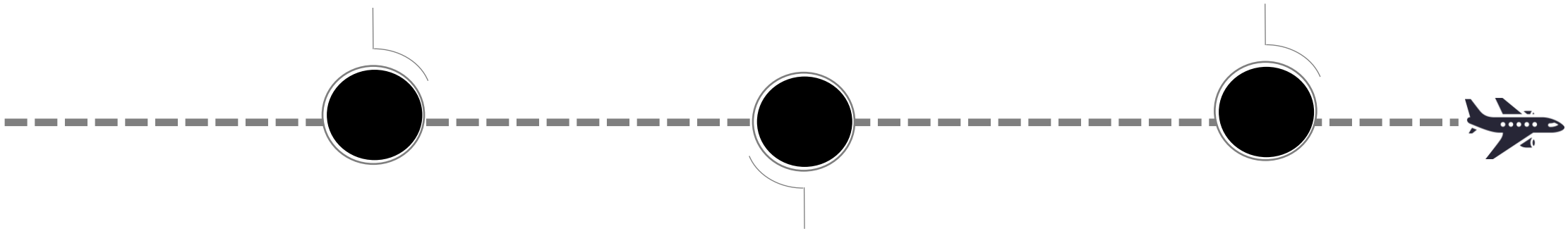


Hydrogen bonding is the main binding forces between chains, it is not all for stacking sheet

Molecular dynamics approach is an effective computer modeling technology

Building the initial structure with cellulose-builder

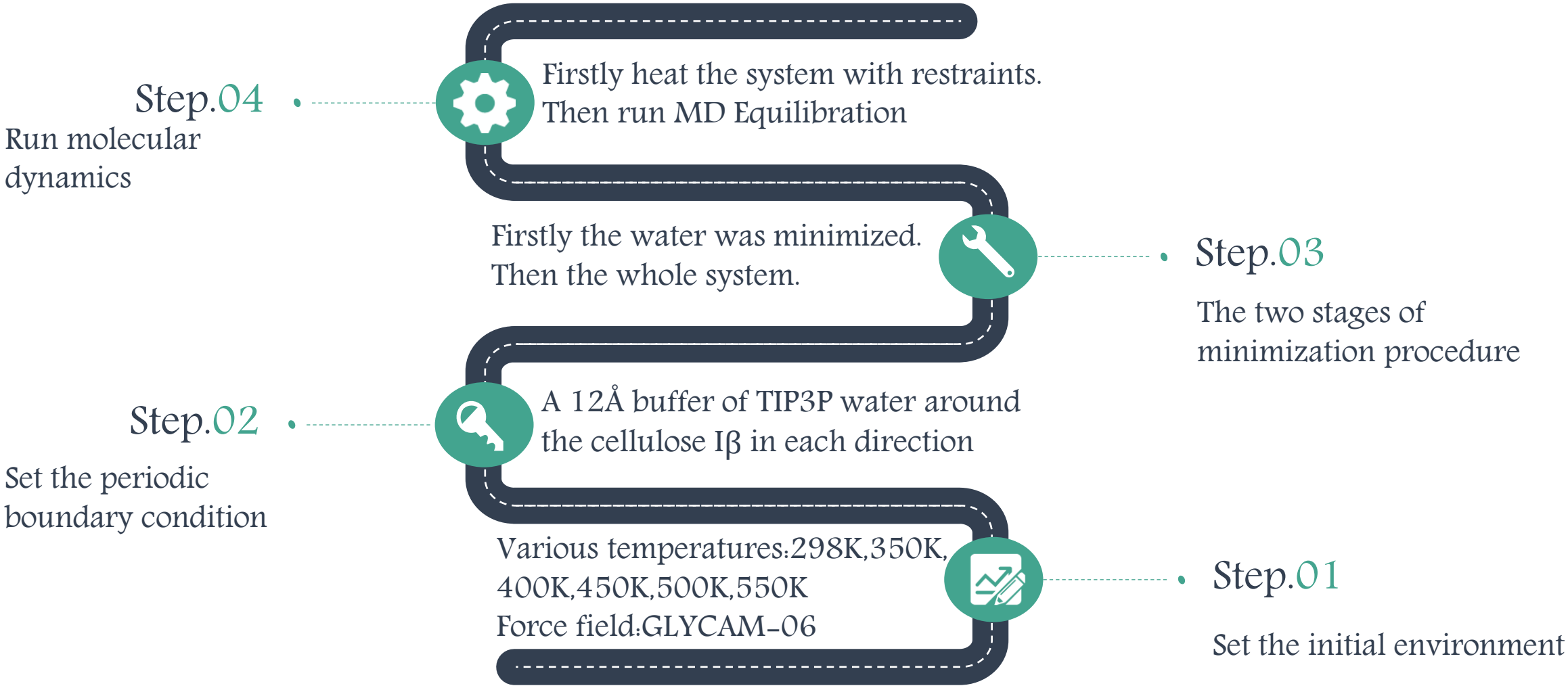
Calculate the interaction energy by program MMPBSA.py of AmberTools



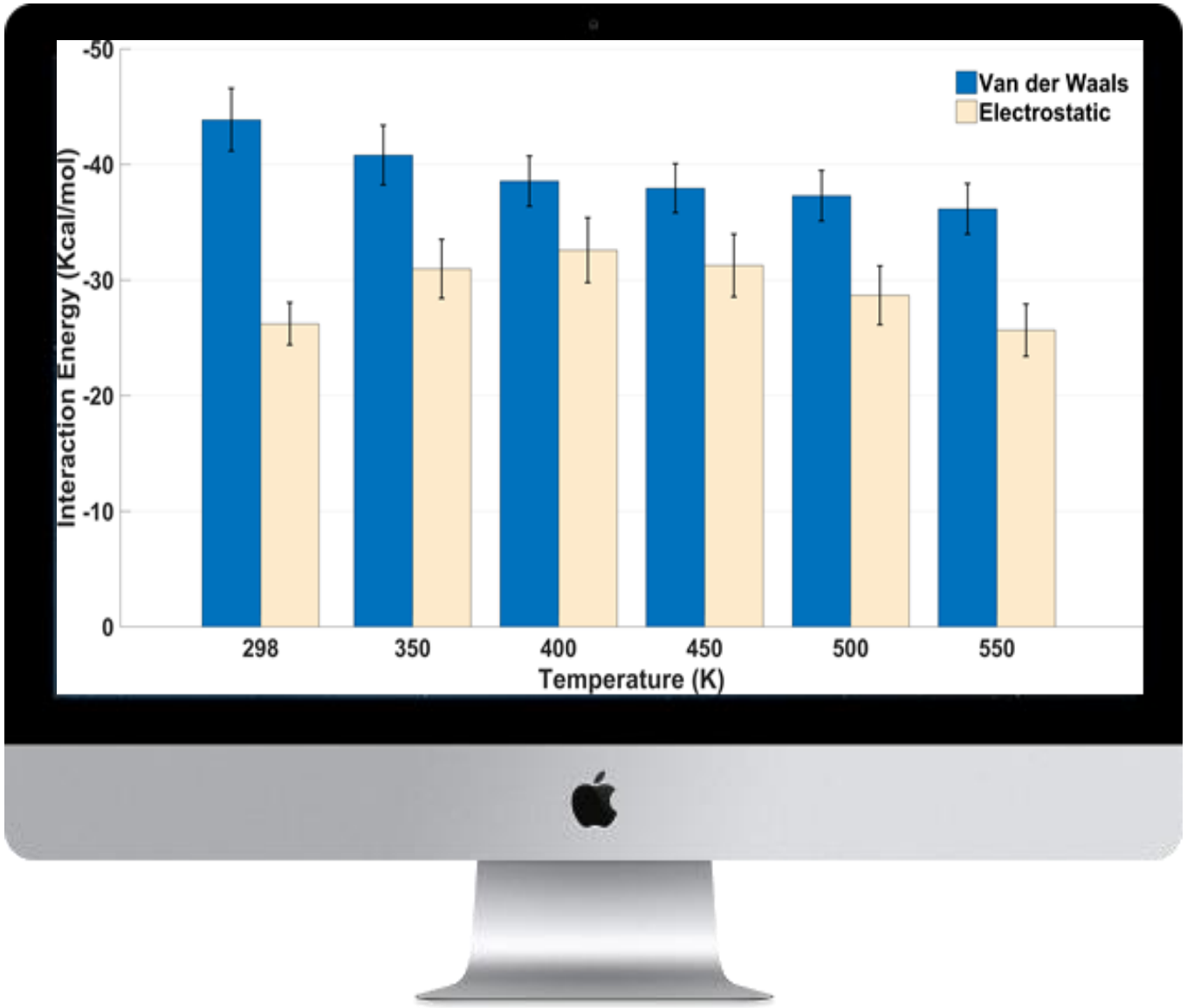
All simulation were performed with Amber software and explicit water

About the initial modeling

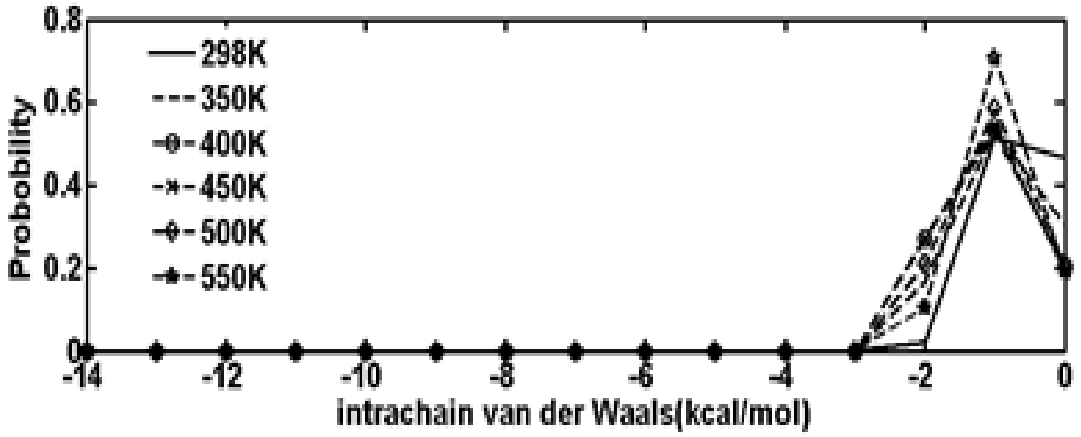
- a = 7.784 Å,b = 8.201 Å, c = 10.38 Å
- α = β = 90° ,γ = 96.5°
- c is the chain direction

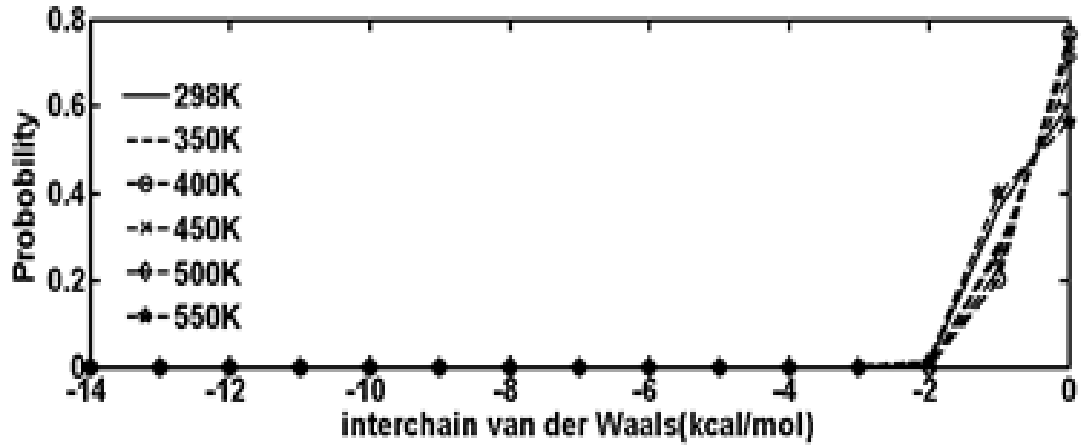


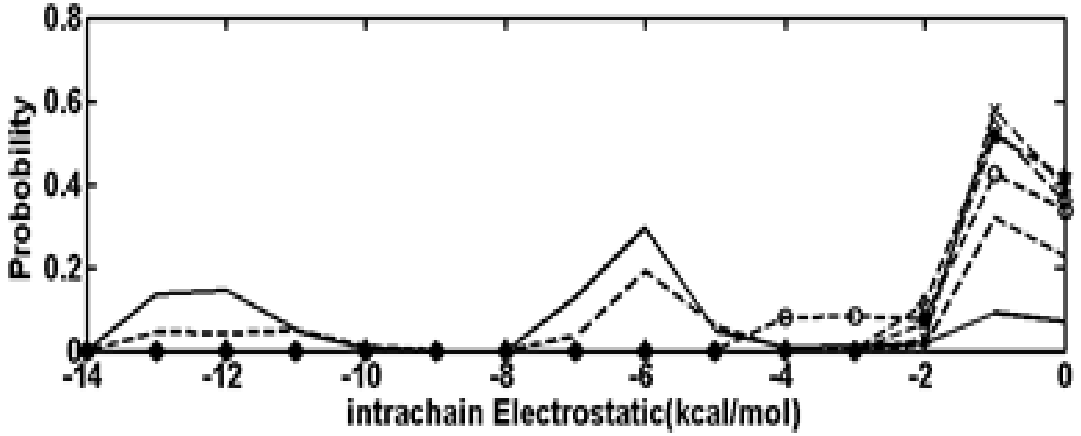
The simulation processing with software Amber

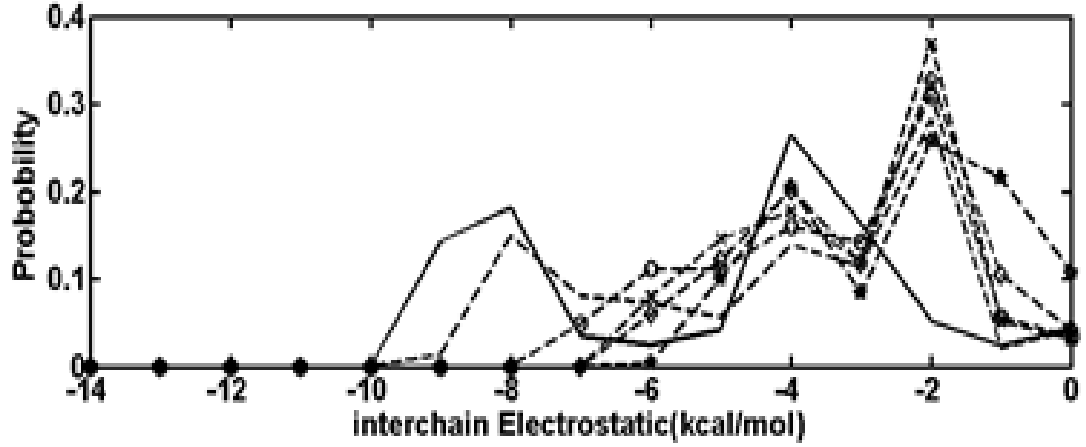


At 298 K, the Van der Waals and electrostatic intermolecular energy per chain are **-43.91 kcal/mol and -26.24 kcal/mol** respectively. The Van der Waals energy gradually **reduces when the temperature rises**, meanwhile the electrostatic energy **increases initially and then decreases.**

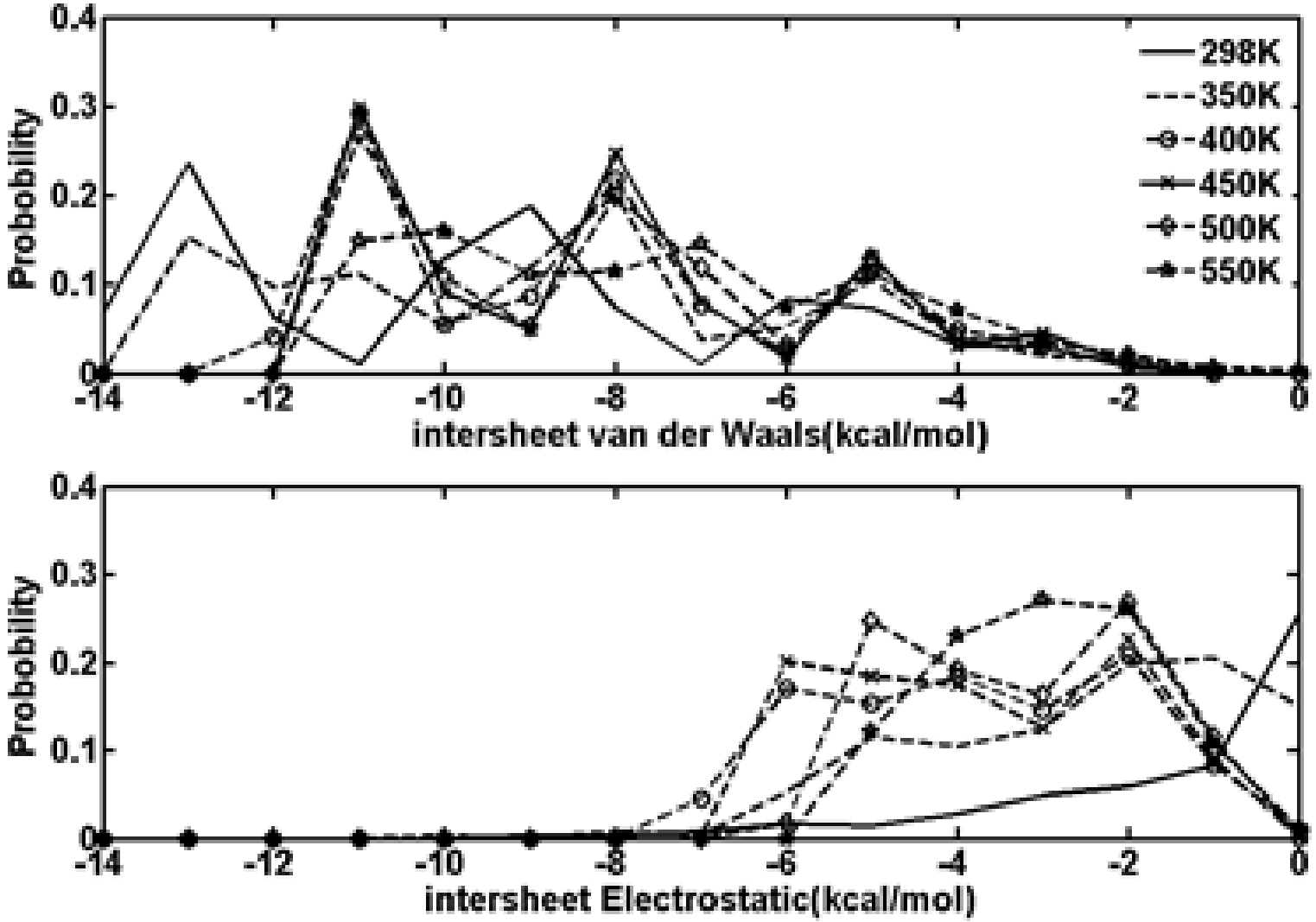




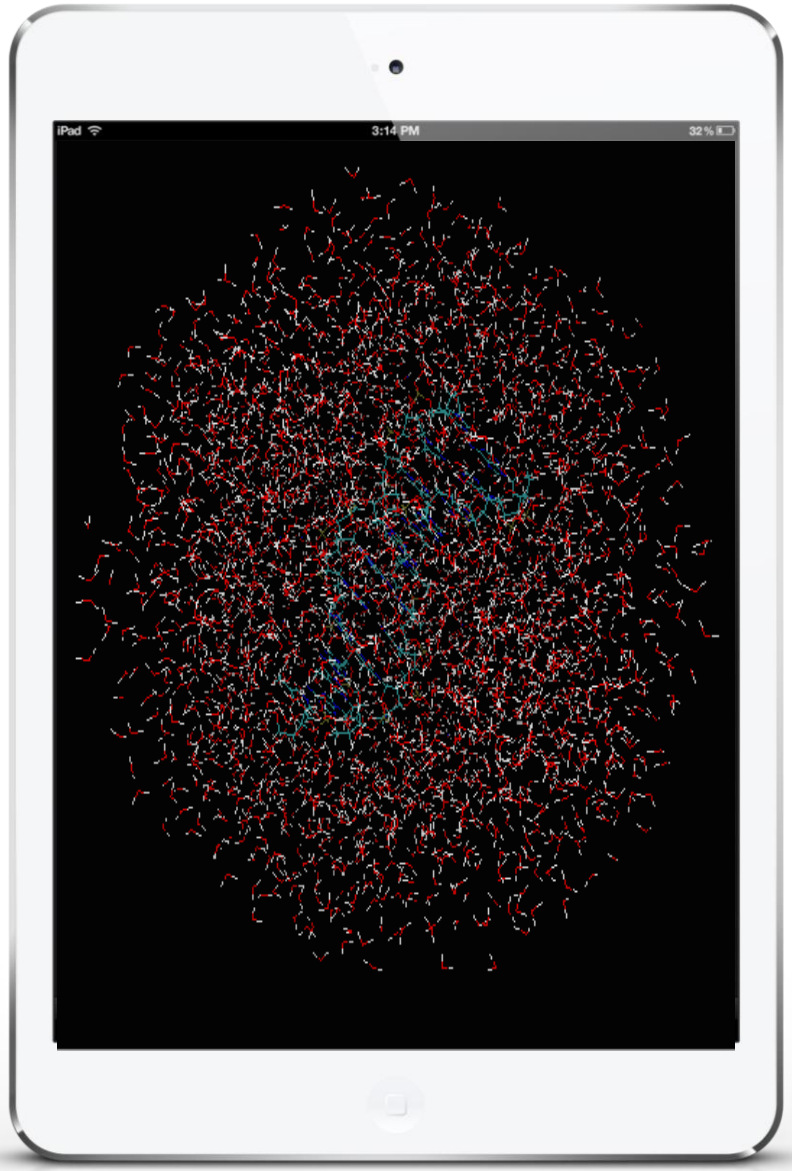




The electrostatic energy of most glucose residues for intrachain lies on **11-14 kcal/mol** and **5-8 kcal/mol**, while located on **7-10 kcal/mol** and **2-5 kcal/mol** at 298 K for interchain. The Van der Waals interaction energy in intrachain **increases slightly** as the temperature rises and there is **almost no growth** for interchain.



The intersheet Van der Waals interaction **decreases slightly** with the temperature **increasing**, The Van der Waals energy of most glucose residues is located on the range of **6-12 kcal/mol** at 550 K.



The interactions were discussed only in water, and no comparison to other solvents. In the next step, we will study the Van der Waals and electrostatic interaction in **different solvent environments**.

THANK YOU .