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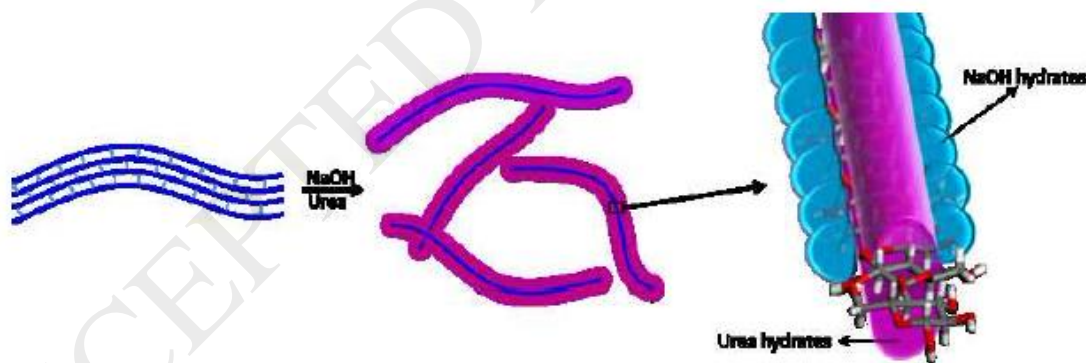
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A molecular dynamics study of cellulose inclusion complexes in

NaOH/Urea aqueous solution

Gang Liu^a, Heng Sun^b, Guokui Liu^c, Heng Zhang^d, Shiling Yuan^d, Qingzeng Zhu^{a,*}^a Key Laboratory of Special Functional Aggregated Materials, Ministry of Education, School of Chemistry and Chemical Engineering, Shandong University, Jinan 250199, P. R. China^b Shandong Siwei Safety Technology Center, Shandong Chemical Industry Research Institute, Jinan250014, P. R. China^c School of Chemistry and Chemical Engineering, Linyi University, Linyi 276000, China^d Key Laboratory of Colloid and Interface Chemistry, Shandong University, Jinan 250199, P. R. China**HIGHLIGHTS**

1. The MD simulation was used to study the cellulose ICs in NaOH–urea aqueous system.
2. All components in cellulose/NaOH/urea aqueous solution were combined in one model.
3. Atomic level scrutiny of spatial structure of cellulose ICs was achieved.
4. The hydrogen bond lifetime was quantitatively estimated in cellulose ICs.
5. Water–water angles distribution in cellulose inclusion complexes was well studied.

GRAPHICAL ABSTRACT**ABSTRACT**

We investigated the dissolution state of cellulose in NaOH/urea aqueous solution using molecular dynamics simulations. All the components, including cellulose, NaOH,

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