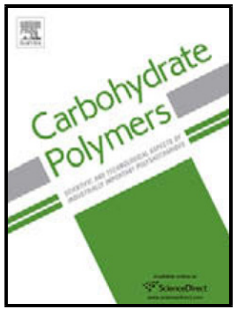

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A molecular dynamics study of cellulose inclusion complexes in NaOH/Urea aqueous solution

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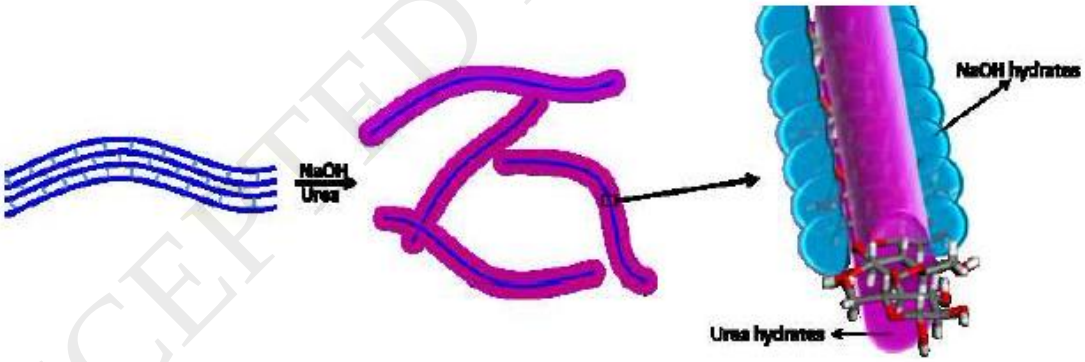
HIGHLIGHTS

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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