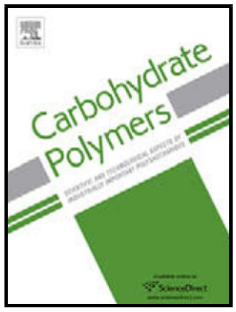

Title: Cellulose nanofiber induced self-assembly of zinc oxide nanoparticles: theoretical and experimental study on interfacial interaction

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Cellulose nanofiber induced self-assembly of zinc oxide nanoparticles: theoretical and experimental study on interfacial interaction

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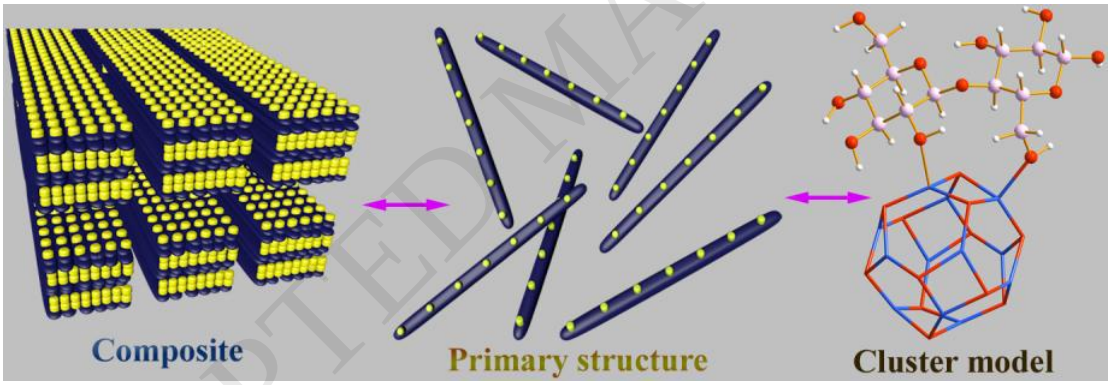
Graphical abstract



The structure-ordered cellulose/zinc oxide composite was experimentally and theoretically explored, which provide an in-depth understanding of interfacial behavior between biopolymer and semiconductor metal oxides and implications for prospective application. It is found that the electrostatic attraction drives the formation of the primary structure and the electron transfer enhances interfacial interaction. It is a dative bond per se and dominated by orbital attractions.

Highlights

- Structure-ordered cellulose/zinc oxide composite was synthesized and calculated by DFT.
- In-depth understanding of interfacial behavior provides implications for experimental synthesis and potential application.