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Modeling of inclusion complexes of amylose and synthetical polymers

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Hierarchical self-assembly of polymers utilizing non-covalent interactions between different molecules represents a versatile approach in the fabrication of functional nanostructured materials. Block copolymers can be regarded as almost ideal building blocks in the construction of large nano-objetcs due to their rapid synthetic accessibility, already large dimensions, tunable aspect ratio etc.

In this respect, hybrid structures of amylose and synthetic polymers are a matter of particular interest owing to the polysaccharide's capability of including certain molecules into its hydrophobic helical cavity [1][2]. For instance, it has been shown that polyethers and polyesters can be complexed in this way [3][4].

In this study we generated computer models of inclusion complexes of amylose and various synthetical polymers in order to investigate differences in their respective complexing abilities. It could be shown that the complexing energies and thus the tendency to form inclusion complexes with amylose correlate with the hydrophobicity of the guest polymer.

References

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