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Structure and molecular interactions of chitin crystallosolvates

Chitin, the second most abundant biopolymer after cellulose, forms crystallosolvates with various small compounds such as water [1] and alcohols [2] as well as amines and organic acids [3]. Over the last decade, a number of high resolution structures of chitin and chitin crystallosolvates have been reported based on X-ray and neutron diffraction techniques [4,5]. Such high-resolution structures have served as a basis for theoretical studies on these crystals to elucidate their molecular interactions. Molecular modelling allows us to understand not only the static crystal structures but also the dynamics of guest molecules in the crystalline lattices [6]. In this contribution, an overview will be given on the crystal structures and molecular interactions in chitin crystallosolvates. The role of intermolecular hydrogen bonds as well as their dynamics will be further discussed based on molecular dynamics and density functional theory calculation studies.

1. J. Blackwell, *Biopolymers* 7 (1969), 281-298.
2. Y. Saito et al., in "Advances in Chitin Science II" (1998), pp. 507-512.
3. Y. Noishiki et al., *Macromolecules* 37 (2004), 6839-6842.
4. Y. Nishiyama et al., *Macromolecules* 44 (2011), 950-957.
5. D. Sawada et al., *Plos One* (2012), e39376.
6. D. Sawada et al., *Cryst. Growth. Des.* 16 (2016) 3345-3352.

Preferred topic

Solid state - crystallosolvates

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