Abstract Submitted
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Ab initio Study of Structure and Hydrogen Bonding of Cellulose Crystals and Surfaces[1] JAMES DAVENPORT, YAN LI, Brookhaven National Laboratory — We have studied the equilibrium structure and hydrogen bonding of cellulose crystals and surfaces using semi-empirical dispersion corrections to density functional theory (DFT+D)[1], which has been shown to be an efficient alternative to more advanced methods for weakly bound aromatic assemblies[2]. The predicted crystal structures for both I_α and I_β phases agree well with experiments. The cohesive energy was decomposed into interchain and intersheet interactions and analyzed in terms of hydrogen bonding and van der Waals dispersion forces. Both interactions were found to be responsible for holding cellulose sheets together. In particular, the dispersion corrections to DFT proved to be indispensable in reproducing the equilibrium intersheet distance and binding strength. Adsorption energy and configuration of water molecules on cellulose surfaces were found to depend sensitively on the surface orientation, adsorption site and contribution from vdW interactions.

[1] S. Grimme, J. Comput. Chem. 27, 1787 (2006).
[2] Y. Li, D. Lu, H-V. Nguyen and G. Galli, J. Phys. Chem. A 114, 1944 (2010).

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