

Ab initio Studies of Crystalline Cellulose

Yan Li

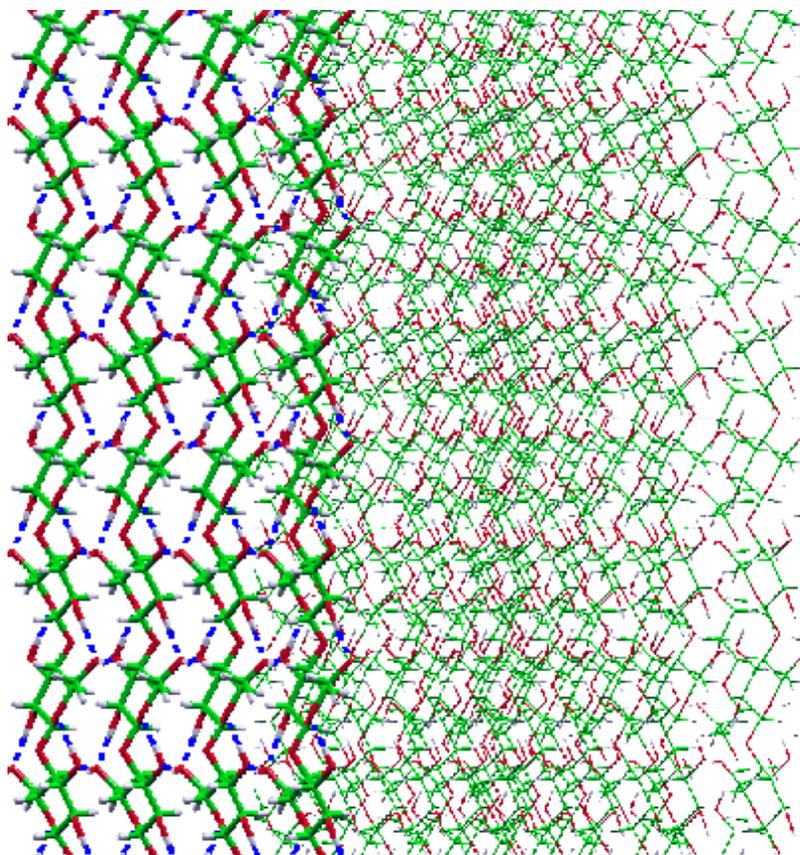
Cellulose, the most abundant carbohydrate biomass on Earth, has attracted widespread attention as a potential alternative energy source. To understand the mechanism of cellulose breakdown and its interaction with the environment, we carried our first-principles studies of the structural, energetic and electronic properties of crystalline cellulose. The crystal structures, cohesive energetics and surface energies predicted from dispersion-corrected density functional theory calculations agree excellently with experiments. Hydrogen bonding and van der Waals dispersion forces are found to be equally important for forming the crystal, despite of the weak nature of the latter. We also investigated the interaction of a single water molecule with the "hydrophobic" $I\beta(100)$ surface. The formation of hydrogen bond at the water/cellulose interface is shown to depend sensitively on the adsorption site, e.g. above the equatorial hydroxyls or the CH moieties pointing out of the cellulose sheets, as well as contributions from dispersion forces.

Presentations and publications

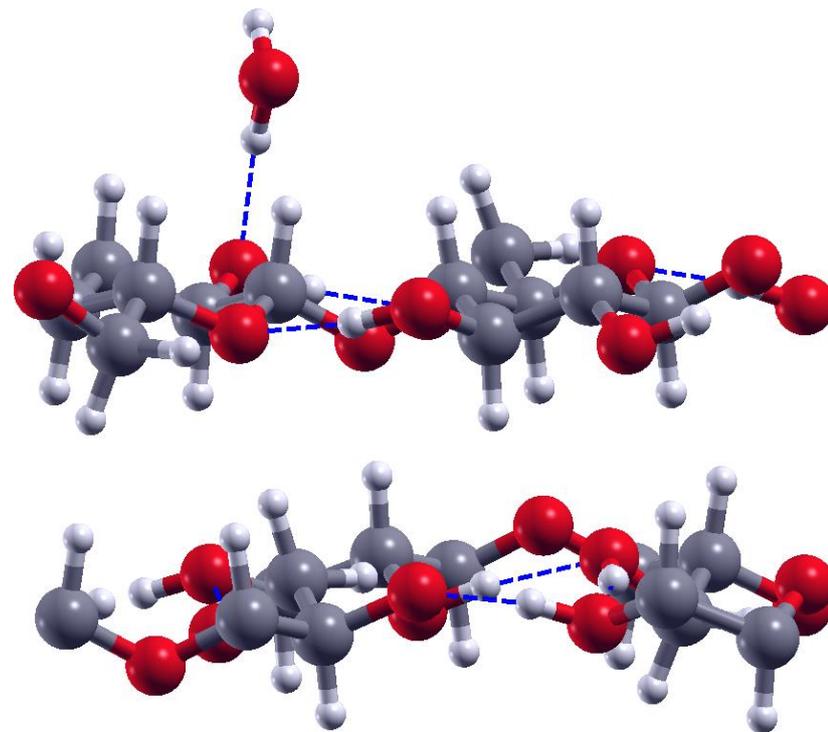
"Ab initio Studies of Cellulose I: Crystal Structure, Intermolecular Forces and Interactions with Water", Yan Li, Milo Lin and James Davenport, J. Phys. Chem. C, accepted.

"Ab initio Studies of Cellulose", presentation at 2011 American Physical Society March Meeting.

"First-Principles Studies of Cellulose I: Crystal Structure, intermolecular interactions and water adsorption", invited seminar at the Laufer Center for Physical and Quantitative Biology, Stony Brook University.



Crystal Structure of Cellulose



Water Adsorption on Cellulose $I\beta(100)$ surface