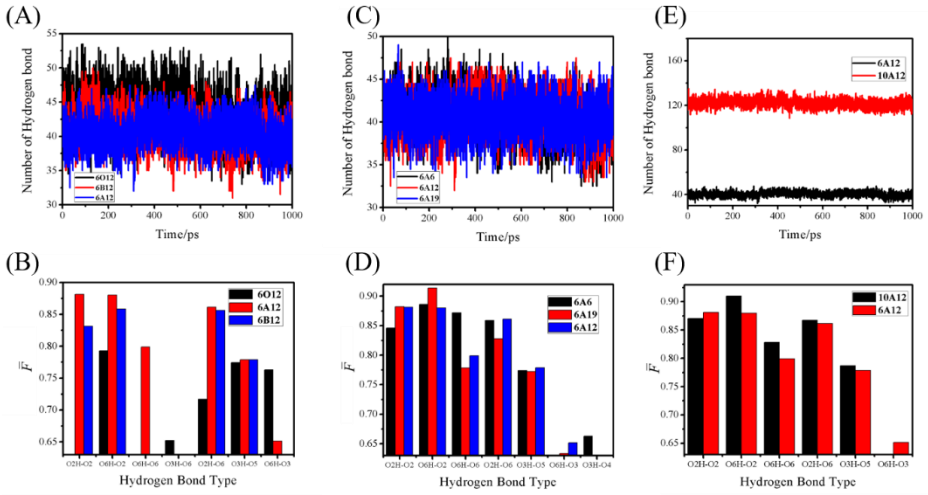
Theoretical Study of Cellulose II Nanocrystals with Different Exposed Facets

Can Leng[1,2,3], Kenli Li[3,4], Zean Tian[4*], Yubing Si[5], Huang Huang[3], Junfeng Li[6], Jie Liu[1,2], Wei-Qing Huang[7], and Keqin Li[4,8***]**

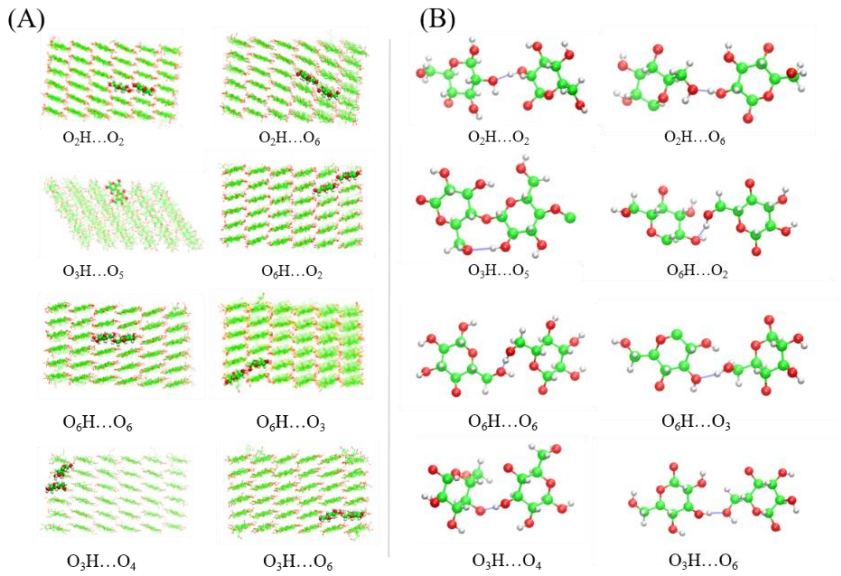
[1]Science and Technology on Parallel and Distributed Processing Laboratory, National University of Defense Technology, Changsha 410073, China
[2]Laboratory of Software Engineering for Complex Systems, National University of Defense Technology, Changsha 410073, China
[3]National Supercomputer Center in Changsha, 410082, China
[4]College of Computer Science and Electronic Engineering, Hunan University, Changsha 410082, China
[5]College of Chemistry, Zhengzhou University, Zhengzhou, 450001, China
[6]College of Chemistry and Chemical Engineering, and Henan Key Laboratory of Function-Oriented Porous Materials, Luoyang Normal University, 471934 Luoyang, China
[7]Department of Applied Physics, School of Physics and Electronics, Hunan University, Changsha 410082, China
[8]Department of Computer Science, State University of New York, New Paltz, New York 12561, USA

*tianzean@hnu.edu.cn
**ybsi@zzu.edu.cn
***lik@newpaltz.edu

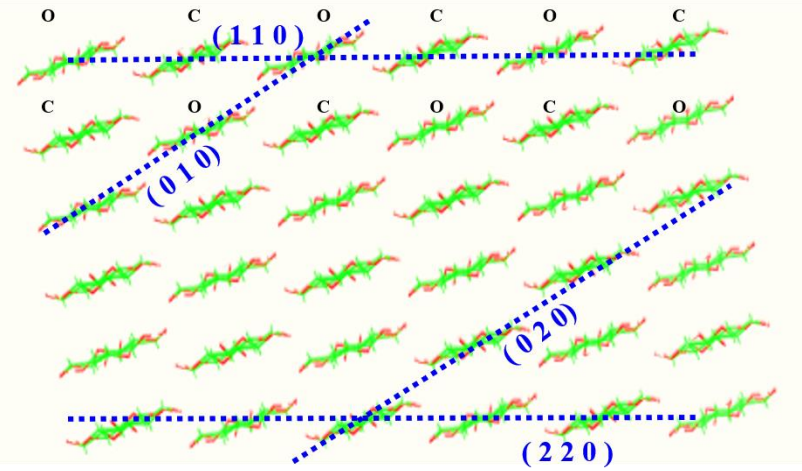
Supplementary Materials:



Supplementary Figure S1. The number and average fraction $\bar{F}$ of hydrogen bonds in the cellulose II nanocrystal models at the terminal anhydroglucose. (A) and (B) are the number and $\bar{F}$ of hydrogen bonds in 6O12, 6A12 and 6B12 of the terminal anhydroglucose, respectively; (C) and (D) are the number and $\bar{F}$ of hydrogen bonds in 6A6, 6A12 and 6A19 models of the terminal anhydroglucose, respectively; (E) and (F) are the number and $\bar{F}$ of hydrogen bonds in 6A12 and 10A12 of the terminal anhydroglucose, respectively.



Supplementary Figure S2. The ONIOM models and the hydrogen bonds scheme. (A) The ONIOM models in which all hydrogen bond types are in their highest fraction samples; (B) The hydrogen bonds are colored with the blue dash line in cellulose II models.



Supplementary Figure S3. The 3×cello-tetramer chain sheet models derived from the original nanocrystal models of cellulose II. O refers to the origin chain, C refers to the center chain. The (0 1 0), (0 2 0) and (1 1 0), (2 2 0) crystal plane are selected with a 3×cello-tetramer chain sheet in both O-C-O, C-O-C types.

Supplementary Table S1. The average hydrogen bond analysis in six types of cellulose II nanocrystal models. The type, average fraction $\bar{F}$ of HBs at the terminal residues, the average O⋯O distance (AvgDist) and angle (AvgAng) of HB type of the six nanocrystal models.

Models	Type	$\bar{F}$	AvgDist/Å	AvgAng/°
6A6	$O_2H\cdots O_2$	0.846	2.766	162.257
	$O_6H\cdots O_2$	0.886	2.756	160.932
	$O_6H\cdots O_6$	0.872	2.777	162.457
	$O_2H\cdots O_6$	0.859	2.769	160.015
	$O_3H\cdots O_5$	0.774	2.756	156.305
	$O_3H\cdots O_4$	0.663	2.771	160.359
6A12	$O_2H\cdots O_2$	0.881	2.764	162.561
	$O_6H\cdots O_2$	0.880	2.755	160.982
	$O_6H\cdots O_6$	0.799	2.782	162.645
	$O_2H\cdots O_6$	0.861	2.769	159.775
	$O_3H\cdots O_5$	0.779	2.752	155.918
	$O_6H\cdots O_3$	0.652	2.761	161.520
6A19	$O_2H\cdots O_2$	0.882	2.763	162.709
	$O_6H\cdots O_2$	0.914	2.751	161.521
	$O_6H\cdots O_6$	0.779	2.777	162.669
	$O_2H\cdots O_6$	0.828	2.767	159.719
	$O_3H\cdots O_5$	0.772	2.746	155.479
	$O_6H\cdots O_3$	0.634	2.804	159.806
10A12	$O_2H\cdots O_2$	0.871	2.764	162.392
	$O_6H\cdots O_2$	0.910	2.754	161.209
	$O_6H\cdots O_6$	0.828	2.776	162.800
	$O_2H\cdots O_6$	0.867	2.765	159.811
	$O_3H\cdots O_5$	0.787	2.750	155.662
6B12	$O_2H\cdots O_2$	0.831	2.769	162.068
	$O_6H\cdots O_2$	0.858	2.758	160.197
	$O_2H\cdots O_6$	0.856	2.768	160.909
	$O_3H\cdots O_5$	0.779	2.763	156.275
6O12	$O_6H\cdots O_2$	0.793	2.757	161.494
	$O_3H\cdots O_6$	0.652	2.798	158.006
	$O_2H\cdots O_6$	0.717	2.791	157.030
	$O_3H\cdots O_5$	0.774	2.768	155.736
	$O_6H\cdots O_3$	0.763	2.740	159.833

Supplementary Table S2. Hydrogen bond type in different cellulose II nanocrystal models.

	6A6	6A12	6A19	10A12	6B12	6O12
$O_2H…O_2$	●	●	●	●	●	
$O_2H…O_6$	●	●	●	●	●	●
$O_3H…O_5$	●	●	●	●	●	●
$O_6H…O_2$	●	●	●	●	●	●
$O_6H…O_6$	●	●	●	●		
$O_6H…O_3$		●	●			●
$O_3H…O_4$	●					
$O_3H…O_6$						●