

Supplementary Material 5: Comparing peak intensities of cellulose peaks – LOI and HBI

Spatiotemporal dynamics of cellulose during enzymatic hydrolysis studied by infrared spectromicroscopy

Tina Jeoh^{1,*}, Jennifer Danger Nill^{1,2,§}, Wujun Zhao^{3,4,§}, Sankar Raju Narayanasamy^{3,5,§}, Liang Chen^{3,6}, and Hoi-Ying N. Holman^{3,*}

[§]These authors contributed equally to this manuscript

¹Biological and Agricultural Engineering, University of California Davis, Davis, CA

²Current: Amyris, Emeryville, CA

³Berkeley Synchrotron Infrared Structure Biology (BSISB), Lawrence Berkeley National Lab (LBNL), Berkeley, CA

⁴Current: Genus IntelliGen Technologies, Windsor, Wisconsin

⁵Current: Biosciences and Biotechnology Division, Physical and Life Science, Lawrence Livermore National Laboratory, Livermore, CA

⁶Current: TikTok, Mountain View, California

*Corresponding Authors

Lateral Order Index (LOI)

The lateral order index (LOI) is calculated as the ratio of peak intensities at 1429 cm^{-1} and 896 cm^{-1} (Figure S5. 1). The ‘amorphous cellulose’ signal at $\sim 896\text{ cm}^{-1}$ is consistently near zero such that the $\text{LOI} \gg 1$.

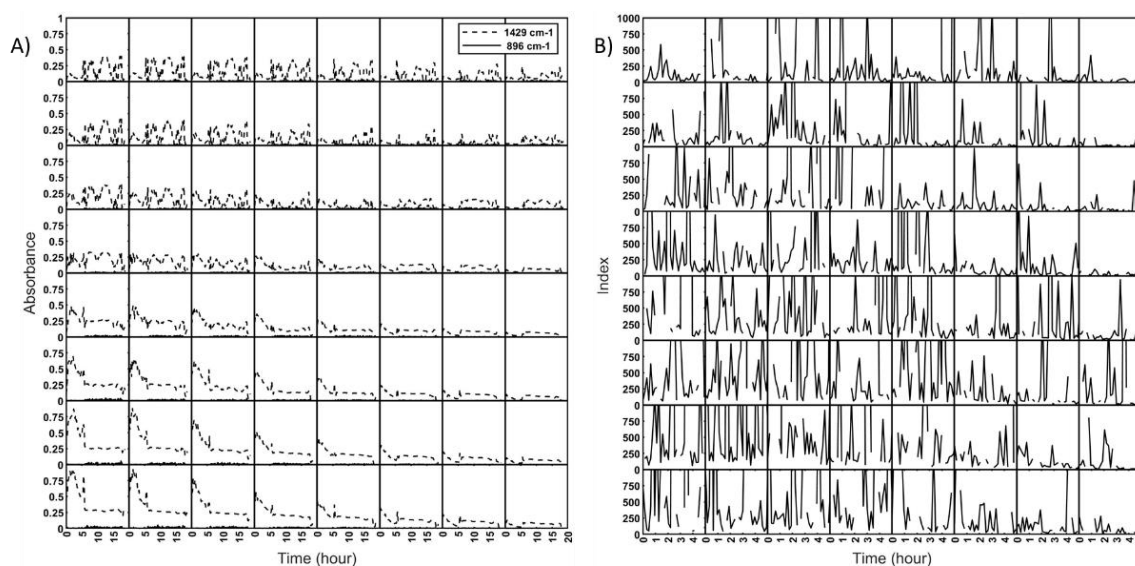


Figure S5. 1: (A) Peak intensities at 1429 cm^{-1} and 896 cm^{-1} over full time course, (B) LOI ($1429\text{ cm}^{-1}/896\text{ cm}^{-1}$).

Hydrogen Bonding Index (HBI)

An alternate assessment of the hydrogen bonding index (HBI) is to take the ratio of the peak intensities at 3345 cm^{-1} and 1429 cm^{-1} . This assessment of HBI compares the intensity of the vibration peak of the hydrogen bonds that C6-O6H participates in (3345 cm^{-1}) and the bending peak of C6-O6H (1429 cm^{-1}). The 1429 cm^{-1} peak, also used in assessing LOI, is associated with the δOH of C6-O6H. Comparing the signal due to hydrogen bonds that the C6-O6H participates in and the signal due to bending of the C6-O6H indicated a steeper decrease in the abundance of the C6-O6H bond than in hydrogen bonding by these bonds. Similar increasing trends in the ratios at the particle edges were thus observed as HBI (Figure 9D in the main manuscript)

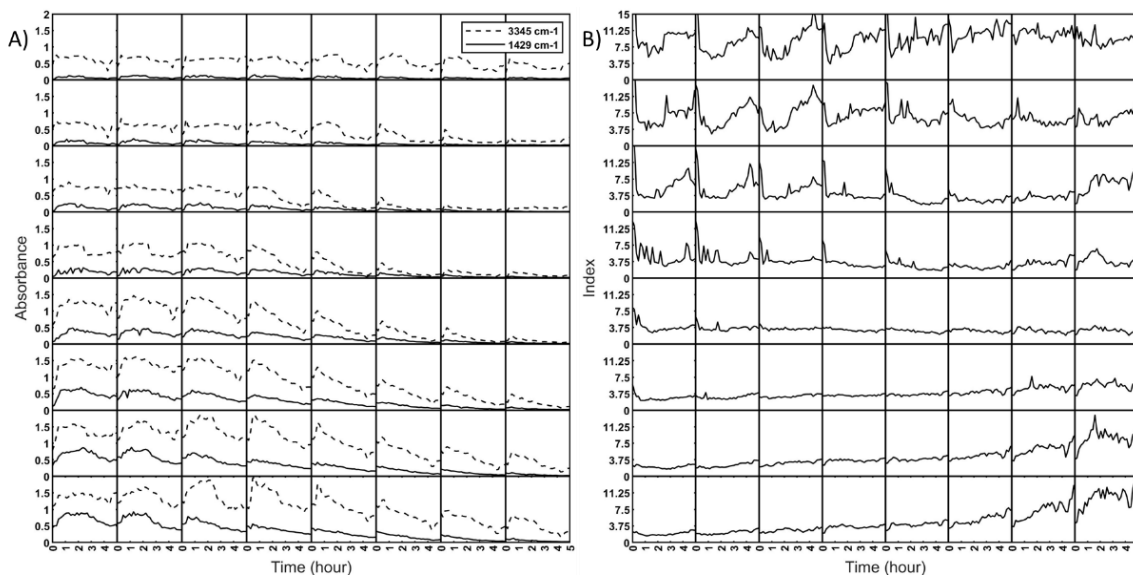


Figure S5. 2: (A) Peak intensities at 3345 cm^{-1} and 1429 cm^{-1} over first 5 hours, (B) HBI ($3345\text{ cm}^{-1}/1429\text{ cm}^{-1}$).