

Electronic Supplementary Information

Molecular insight into cellulose regeneration from cellulose/ionic liquid mixture: effects of water concentration and temperature

Krishna M. Gupta, Zhongqiao Hu and Jianwen Jiang*

Department of Chemical and Biomolecular Engineering, National University of Singapore, 117576, Singapore

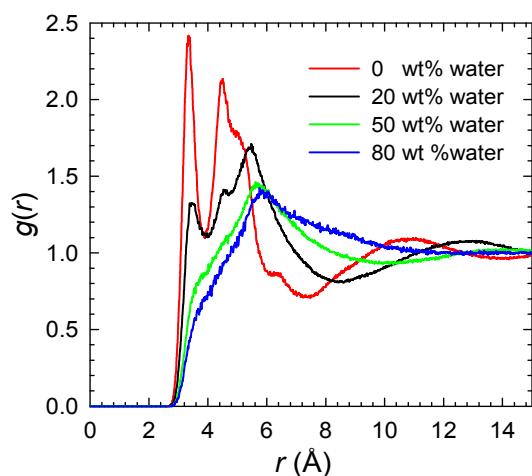


Fig. S1 Radial distribution functions for C_2 atom of $[BMIM]^+$ around O_A and O_B atoms of $[Ac]^-$ in cellulose/ $[BMIM][Ac]$ /water mixtures at 0, 20, 50, and 80 wt% water.

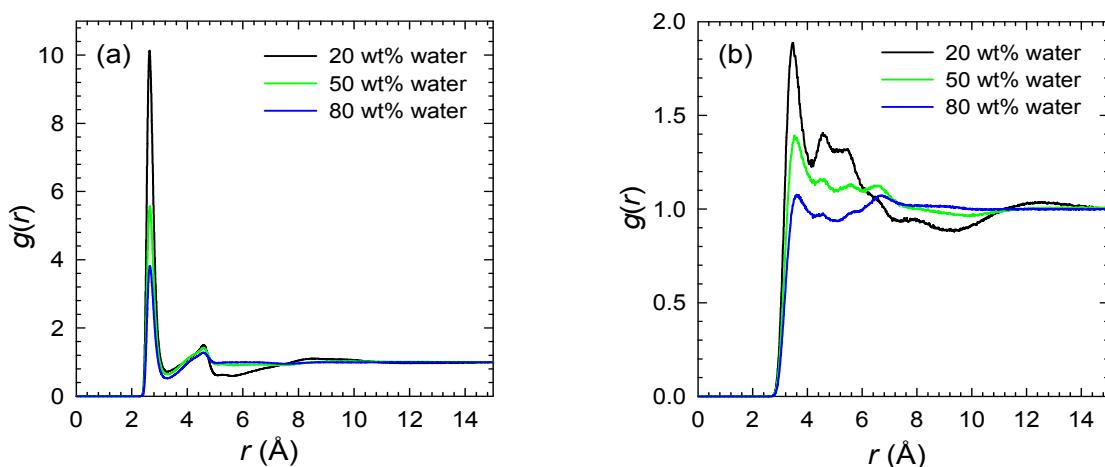


Fig. S2 Radial distribution functions for O_w atom of water around (a) O_A and O_B atoms of $[Ac]^-$ (b) C_2 atom of $[BMIM]^+$ in cellulose/ $[BMIM][Ac]$ /water mixtures at 20, 50, and 80 wt% water.

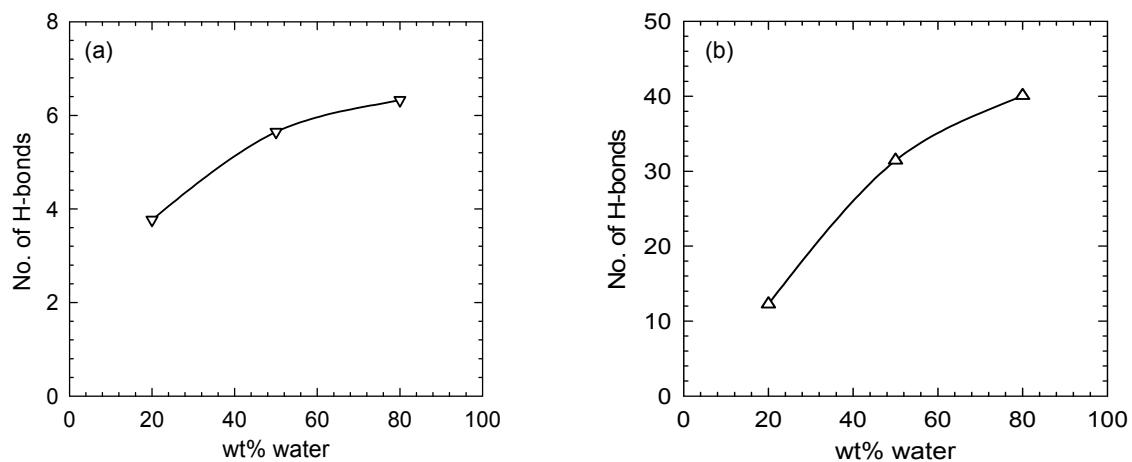


Fig. S3 Numbers of H-bonds between (a) $[\text{Ac}]^-$ -water per $[\text{Ac}]^-$ (b) cellulose-water per cellulose in cellulose/[BMIM][Ac]/water mixtures at 20, 50, and 80 wt% water.