XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

A Computational Study of The Wetting of Nanocrystalline Cellulose

Lucas N. Trentin, Munir S. Skaf

Institute of Chemistry, University of Campinas, Barão Geraldo, 13083-852, Campinas - São Paulo, Brazil.

Abstract: Sugarcane lignocellulosic biomass is a promising material, being the most available resource for biofuel generation [1]. Its recalcitrance to enzymatic hydrolysis is a key factor to overcome in order to have an economically viable conversion of plant biomass in fermentable sugars [2]. Molecular dynamics (MD) simulations have been used to model water nanodroplets on crystalline cellulose in order to study the hydrophilicity of cellulose faces. Cellulose builder [3] and Packmol [4] were used to create (010), (110), (1-10) and (100) cellulose Iβ faces packed with 3000 water molecules. Three 40ns independent MD simulations using CHARMM force field gave a droplet profile for each face, which was analyzed with LBADSA [5] plugin for ImageJ. It was found that (010) and (110) faces where completely wetted, whereas in (1-10) and (100) faces, contact angles close to 30^{o} where observed, showing that even the so called "hydrophobic surfaces" exhibit some hydrophilic behavior. Full and partial wetting where associated with exposure of hydroxyl groups and axial aliphatic hydrogen atoms, respectively. In addition, the developing of a new software for contact angle determination and study of modified cellulose surfaces are planned to happen in the following months. These data can be useful for biotechnological applications.

Key-words: Crystalline Nanocellulose, Molecular Dynamics, Hydrophilicity, Contact Angle.
Support: This work has been supported by CNPq (144359/2017-0) and FAPESP (2013/08293-7).

References:

[1] S. P. S. Chundawat, G. T. Beckham, M. E. Himmel, B. E. Dale, Annu. Rev. Chem. Biomol. Eng., 2, 121 (2011).
[2] Y. H. P. Zhang, M. E. Himmel, J. R. Mielenz, Biotechnol. Adv. 24, 452 (2006).
[3] T. C. Gomes, M. S. Skaf, J. Comput. Chem. 33, 1338 (2012).
[4] L. Martínez, R. Andrade, E. G. Birgin, J. M. Martínez, J. Comput. Chem. 30, 2157 (2009).
[5] A. F. Stalder, T. Melchior, M. Müller, D. Sage, T. Blu, M. Unser, Colloids Surf., A 286, 92 (2010).