

Examining the use of Nanocellulose Composites for the Sorption of Contaminants of Emerging Concern: An Experimental and Computational Study

*Jairo Herrera-Morales^{1,2}, Kathleen Morales², Damarys Ramos^{1,2}, Edwin O. Ortiz-Quiles^{1,2}, Juan M. López-Encarnación³, and Eduardo Nicolau^{*1,2}*

¹ Department of Chemistry, University of Puerto Rico, Rio Piedras Campus, PO Box 23346, San Juan, Puerto Rico USA 00931-3346

² Molecular Sciences Research Center, University of Puerto Rico, 1390 Ponce De Leon Ave, Suite 2, San Juan Puerto Rico USA 00931-3346

³ Department of Mathematics-Physics, University of Puerto Rico, Cayey Campus, Cayey, Puerto Rico USA 00736

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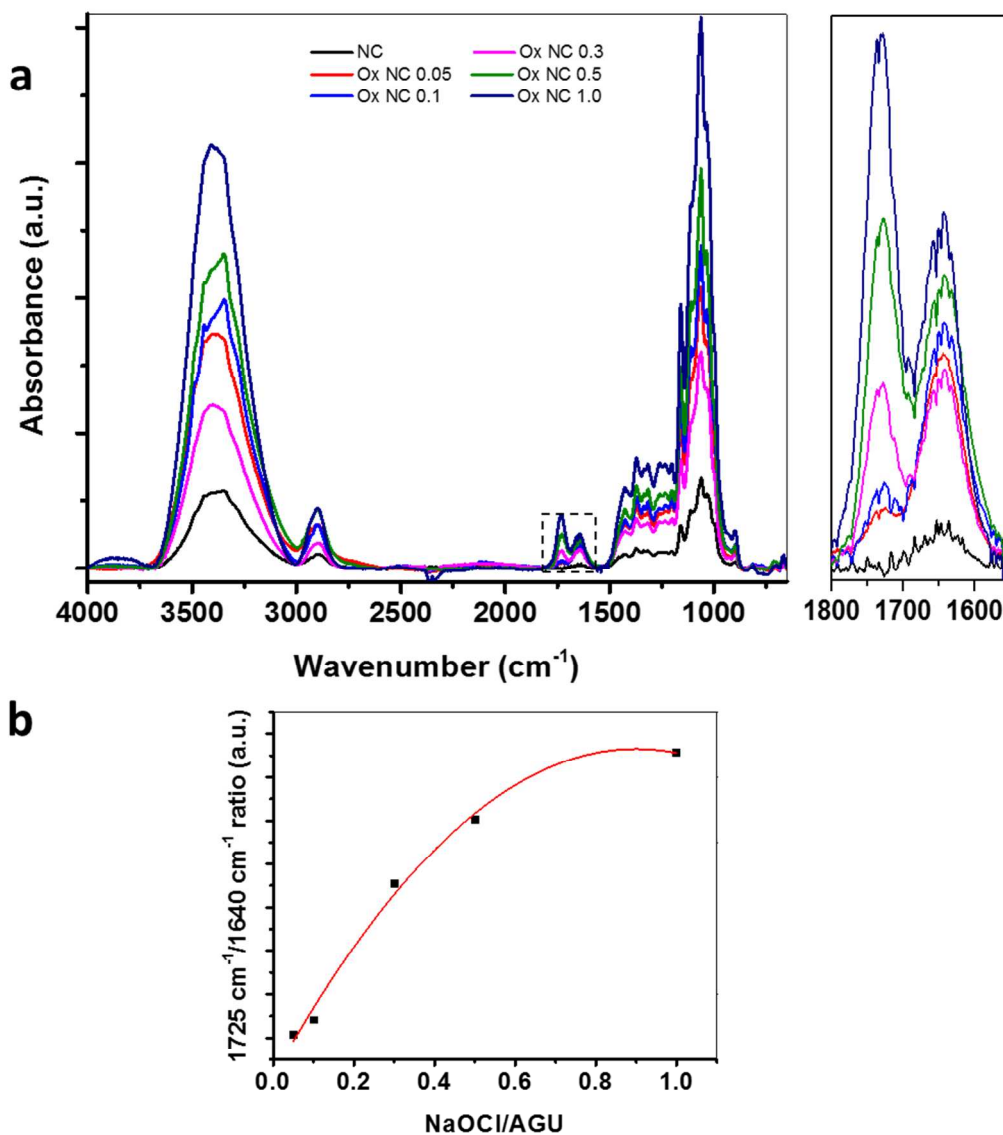


Figure S1. a) FTIR spectra of NC and oxidized NC using 0.05-1.0 NaOCl/AGU molar ratios. The highlighted area corresponds to the carbonyl and adsorbed water bands. b) Plot of the 1725 cm^{-1} /1640 cm^{-1} height ratios as a function of NaOCl/AGU molar ratios.

Fourier transform infrared (FTIR) spectra of NC, and oxidized NC using 0.05-1.0 NaOCl/AGU molar ratios Thermo Scientific Nicolet IS 50, FTIR Continuum microscope. The spectral width ranged from 600-4000 cm^{-1} , with a resolution of 4 cm^{-1} , an accumulation of 64 scans. Samples were prepared in a diamond

window cell to obtain a thin film of the material. Spectra were converted from transmittance to absorbance using the equation:

$$A = 2 - \log \%T$$

Where A is the absorbance and $\%T$ is the transmittance percent to obtain the spectra of Fig. 1a. Ratios of the band around 1725 cm^{-1} corresponding to the carboxylic acid stretching and the band at 1640 cm^{-1} corresponding to the adsorbed water were calculated for all of the TEMPO oxidized samples. The values were plotted as a function of the NaOCl/AGU molar ratios as seen in Fig. 1b.

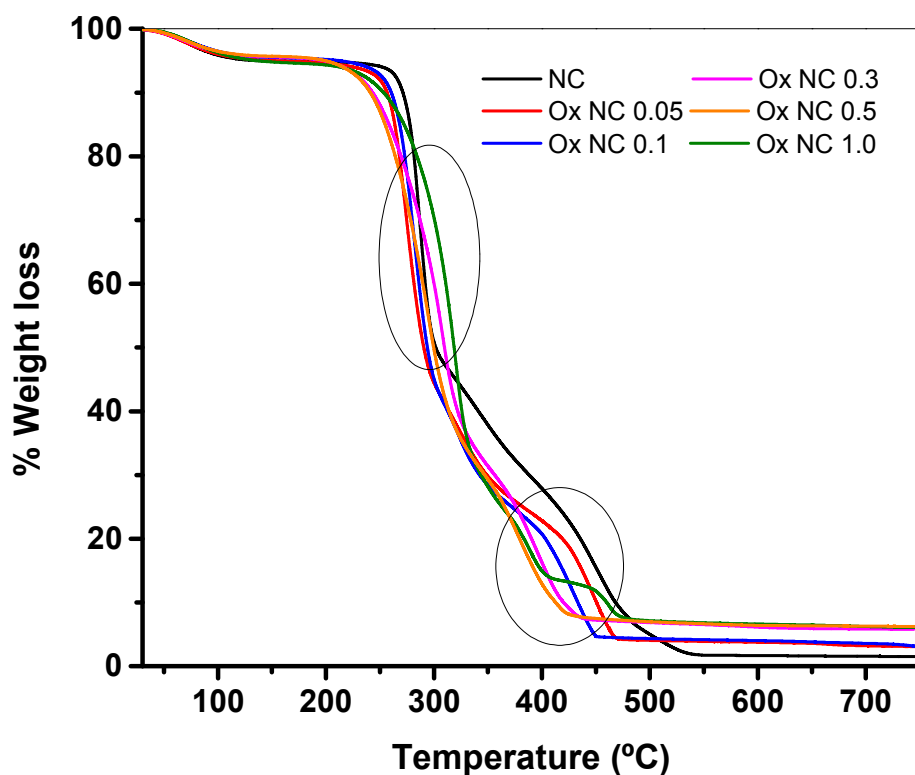


Figure S2. Thermograms of NC and oxidized NC using 0.05-1.0 NaOCl/AGU molar ratios.

Thermograms of NC and oxidized NC were recorded with a Perkin-Elmer STA 6000 simultaneous thermal analyzer. For the analysis 10 mg of sample were weighted in a ceramic crucible and heating from 30-750°C with a ramp of 20°C/min under air atmosphere at a constant flow rate of 20 ml/min.

Thermograms of NC samples TEMPO-oxidized with different NaOCl/AGU molar ratios were compared to NC. In all of the cases the thermostability of NC were affected, particularly, oxidized NC obtained from NaOCl/AGU molar ratios of 0.5 and 1.0, which presented major variations in the hierarchical degradation patterns as showed in the circled areas.

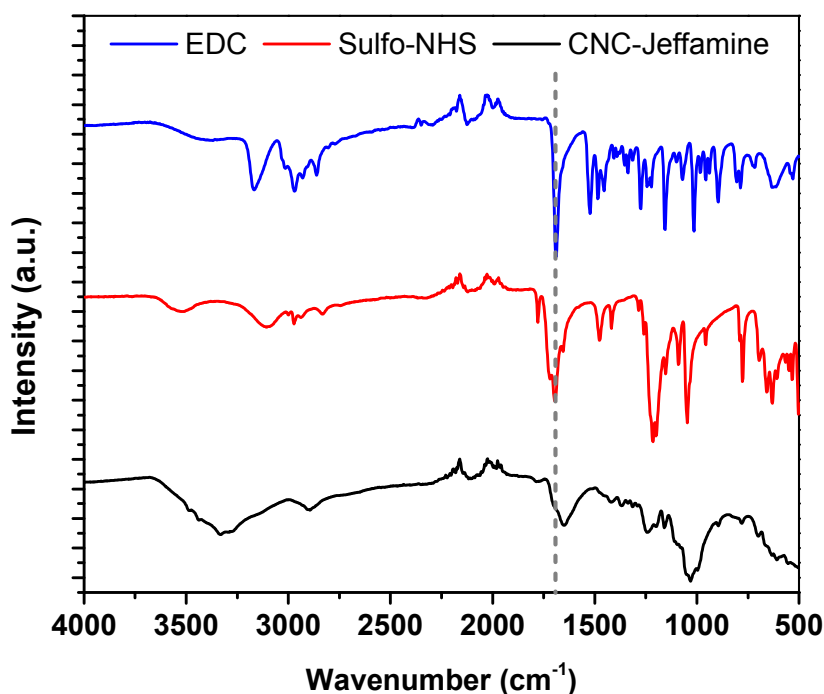


Figure S3. FTIR spectra of N-(3-Dimethylaminopropyl)-N'-ethylcarbodiimide (EDC), N-Hydroxysulfosuccinimide sodium salt (sulfo-NHS), and NC-Jeffamine.

Fourier transform infrared (FTIR) spectra of EDC, sulfo-NHS, and NC-Jeffamine were recorded on a Bruker Tensor 27 using attenuated total reflectance mode (ATR). The spectral width ranged from 500-4000 cm⁻¹, with a resolution of 4 cm⁻¹, an accumulation of 32 scans.

FTIR spectra of Fig. S3 highlight the possible contribution of the bands around 1700 cm^{-1} to the shoulder of the band with the peak around 1650 cm^{-1} in the FTIR spectra of NC-Jeffamine.

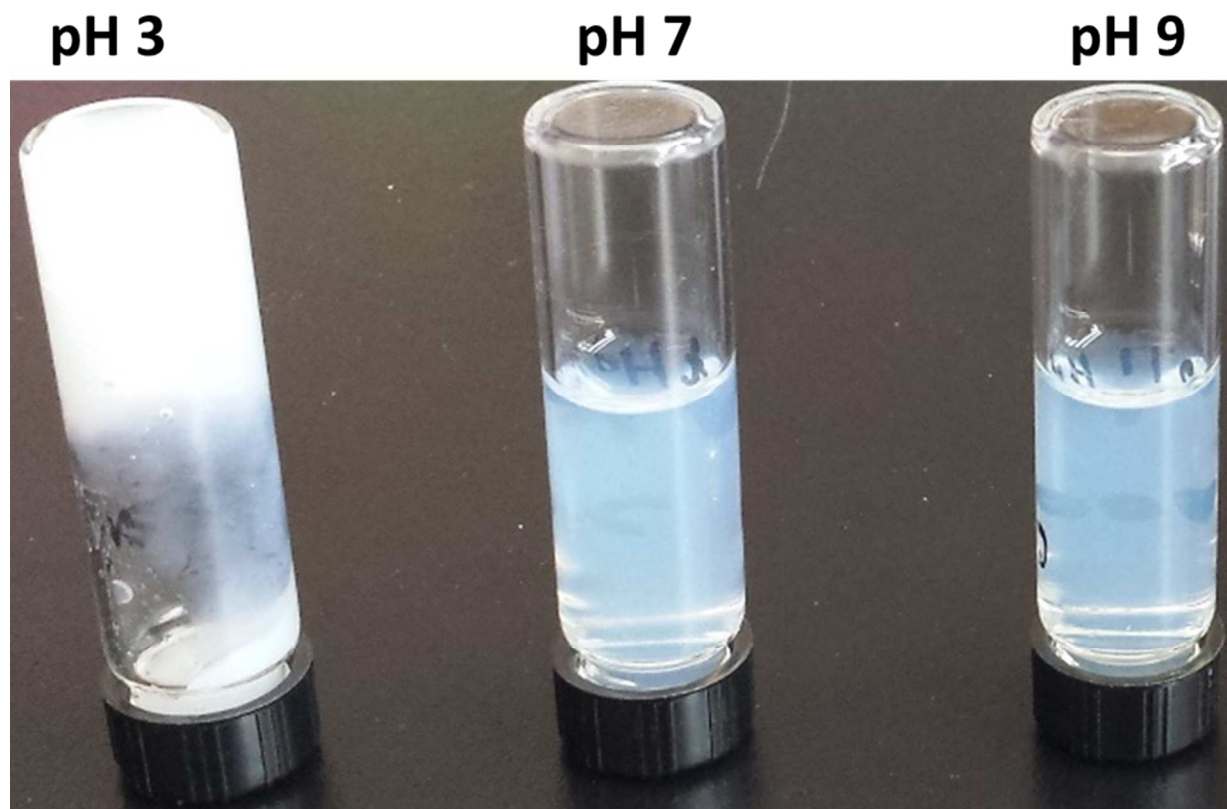


Figure S4. NC-Jeffamine aqueous suspensions at different pHs.

Fig. S4 shows 1% wt. aqueous suspensions of NC-Jeffamine at pH 3, 7, and 9. As the pH increases the dispersion of the NC-Jeffamine particles increases as well. This phenomenon is associated with the deprotonation of carboxylic acid that remained in the NC surface after the Jeffamine grafting reaction. Deprotonation produces negatively charged carboxylates that promotes electrostatic repulsions between the particles in the aqueous solutions. On the other hand, acidic pH maintain the protonated form of the carboxyl groups. At this point, the particles in the solutions prefer to be aggregated due to the formation

of H-bonds. At this pH the suspension is viscous enough to form a gel that keeps in the bottom of the vials even at upside down position.

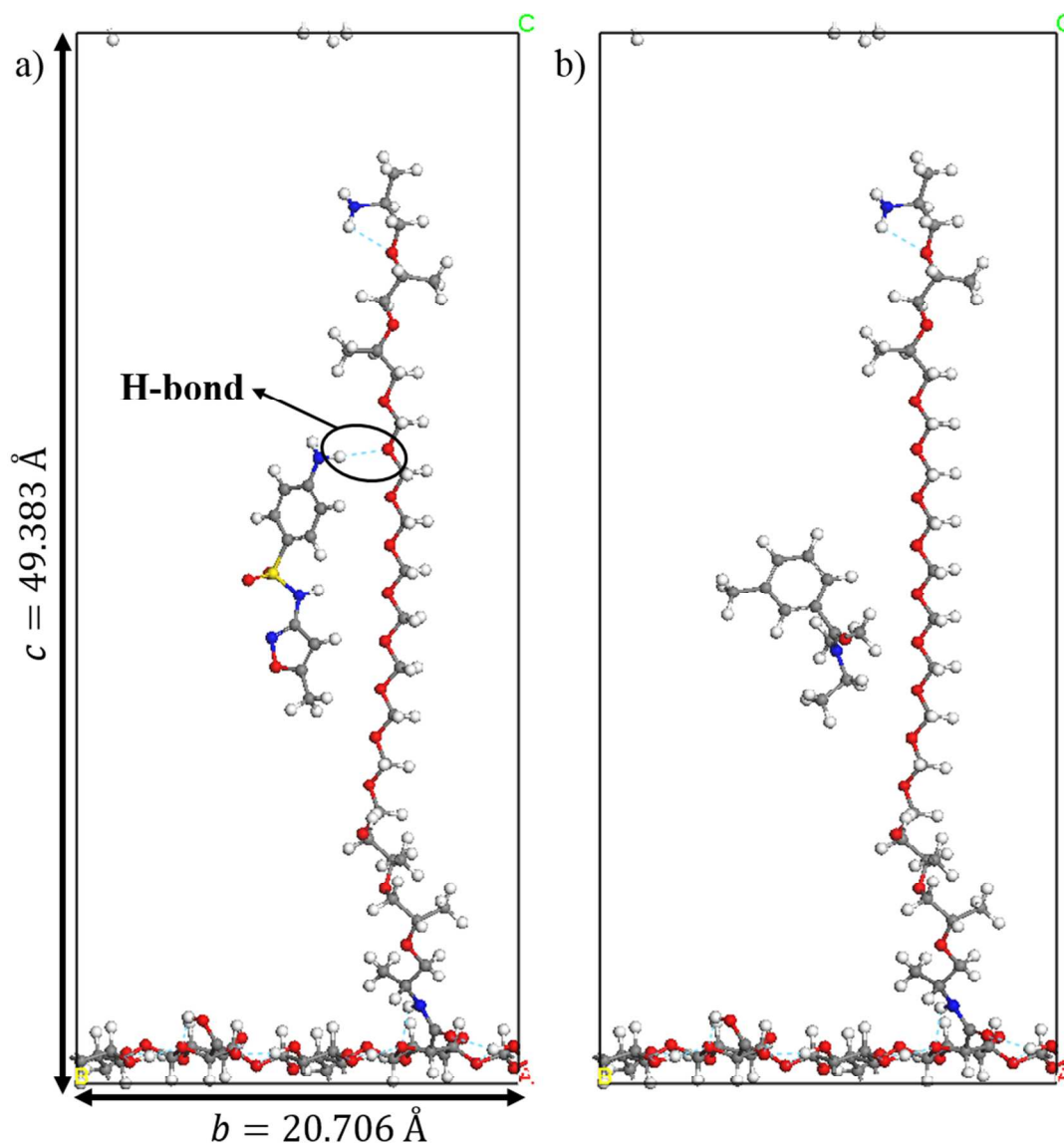


Figure S5. Atomic structures models for unit-cell representation of minimum-energy structures for (a) Sulfamethoxazole and (b) DEET adsorbed on NC-Jeffamine.

Fig. S5 shows the optimized (minimum-energy) structures for adsorbate Sulfamethoxazole and DEET on NC-Jeffamine. The binding energies for sulfamethoxazole and DEET on NC-Jeffamine are 14.32 kcal/mol and 8.37 kcal/mol, respectively.