

# Optimization of polymeric nanomaterials for biomedical applications using computational simulation

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## Abstract

An innovative approach is used to develop nanopolymeric fibrous materials with optimized porosity and thickness. Using our own materials simulator we are able to design a new material with optimized properties for biomedical applications. The material optimization is fundamental for obtaining functionalities like the transport of molecules, support and structure coating [1]. The use of a validated computational simulator is an important tool to optimize structural properties [2-3]. In this study nanofibers of polyamide-6 and polyvinyl alcohol were prepared by electrospinning which is a technique that allows the creation of fibers with diameters down to nanoscale. We have used scanning electron microscopy to measure fiber dimensions, porosity and thickness. Using 60 SEM images, and selecting 20 fiber and 25 pores per image, we have obtained an average value of fiber diameter and pores, for polyvinyl alcohol  $352 \pm 2.6 \text{ nm}$  and  $1.29 \pm 0.0068 \mu\text{m}$  and for polyamide-6  $381 \pm 2.2 \text{ nm}$  and  $1.23 \pm 0.0060 \mu\text{m}$ . The material optimization was done using the computational simulator, adapted to nanoscale. In conclusion, using the experimental characterization and the simulation model for porous materials we were able to simulate and produce a nanomaterial with optimized porosity and thickness.

## References

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- [3] Curto, J.M.R., Hekmaty, A.H., Drean, J.Y., Conceição, E.L.T Portugal A.T.G., Simões, R.M.S., Santos Silva, M.J. In Proc. of the 11th World Textile Conference, Autex2011, Mulhouse, France, **2** (2011) 639-643

## Figures

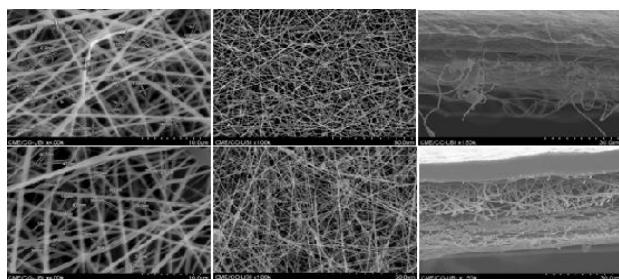


Figure 1: Scanning electron microscopy images of polyvinyl alcohol and polyamide-6. In the top, from right to left, fiber diameter, pore width and thickness, for polyvinyl alcohol structures. The bottom images are fiber diameter, pore width and thickness for polyamide-6 structures.

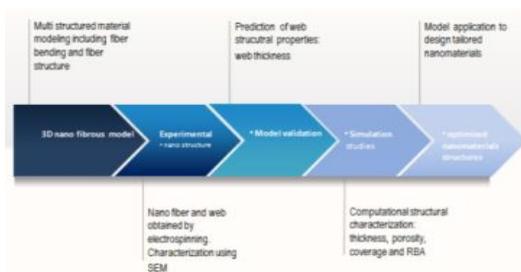


Figure 2: Methodology using simulation and experimental characterization to optimize and develop new porous nanomaterials for biomedical applications.