

Ion Condensation onto Self-Assembled Nanofibers

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Journal of Polymer Science Part B: Polymer Physics 2017, 55, 901-906.

Nanofibers are an increasingly studied topic with potential for drug delivery, as well as tissue and nerve regeneration. They are composed 100% of chemicals naturally produced by the body, allowing for seamless integration. Here, we investigate, via simulation, what happens on the interface between nanofibers and a salt solution. This simplified case allows us to establish a framework for potential interactions within the body, thereby increasing our understanding of what occurs once the nanofiber is placed inside the area of concern. With this model we are able to extrapolate information regarding how salts will play a role in the drug release from the nanofiber, and how tissue might regenerate with this implanted scaffold.

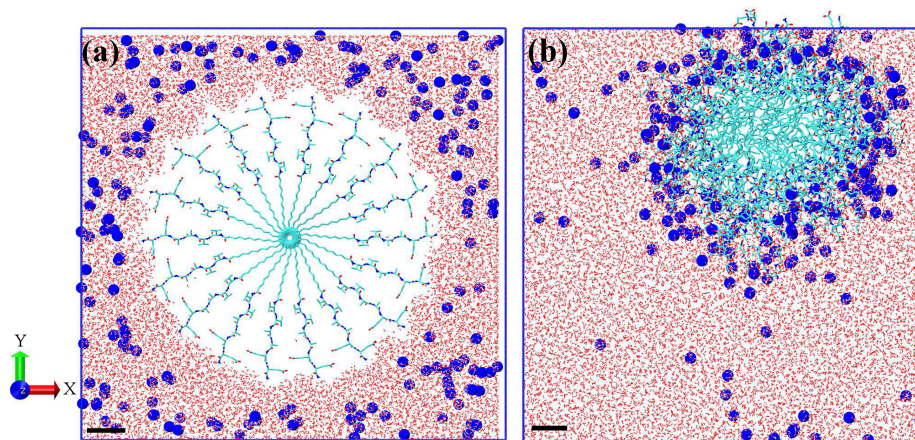


Figure 1: (a) Initial simulation box configuration before performing any runs. (b) Simulation box after finishing 100ns production run, clearly showing ion condensation. Sodium ions are colored blue, water is colored red, and peptides are colored green. Periodic boundary conditions are employed. Scale bar represents 1nm.

Acknowledgements: This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award # DE-FG02-08ER46539 for BQ and MOC (computational studies), and DE-FG02-00ER45810 for JHO (imaging studies). ED-Y thanks the hospitality of the REU program of the Northwestern University Materials Research Science and Engineering Center (NUMRSEC) funded by the NSF under Award No. DMR-1121262. JHO acknowledges an IBNAM-Baxter Early Career Award.