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Ion Condensation onto Self-Assembled Nanofibers ELAD DEISS-YEHIELY, Northwestern University, JULIA ORTONY, Massachusetts Institute of Technology , BAOFU QIAO, Argonne National Laboratory, SAMUEL STUPP, MONICA OLVERA DE LA CRUZ, Northwestern University — Self-assembled peptide amphiphile (PA) nanofibers are a class of supramolecular materials with promising applications in nanotechnology. Alignment of nanofibers, which is essential for biomaterials applications, is achieved by introducing salts to PA nanofiber suspensions. Regardless of its importance, the effect of ion concentrations on the porperties of these nanostructures remains unexplored. Using atomistic molecular dynamics simulations, canonical PA nanostructures are investigated in order to elucidate the relationship between counterion condensation and morphological changes. Simulations reveal that nanofibers with the highest density cross-section have expanded radii. This expansion decreases the accessible volume for sodium counterions and diminishes the counterion translational entropy, while also reducing the total electrostatic potential. Interestingly, we show that the competition between these effects leads to a fraction of condensed counterions independent of the fiber radius.

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