UNRAVELING CELLULOSE FIBERS: A TWISTED TALE

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Abstract

The field of cellulose research stands divided regarding the 3-dimensional structure of cellulose (cotton) microfibrils. Some scientists believe the fibers exist as linear bundles, while others believe the bundles adopt a twisted shape. Experimental evidence exists to support both opinions, but the majority of theoretical data predicts a twisted structure. Members of the GLYCAM force field team have undertaken a project to explore the origin of the twisting phenomenon observed in molecular dynamics simulations from the perspective of force field and simulation methodology. This project aims to understand whether twisted microfibrils are an artifact of theoretical predictions or whether they could be the true state of cellulose bundles in cotton.