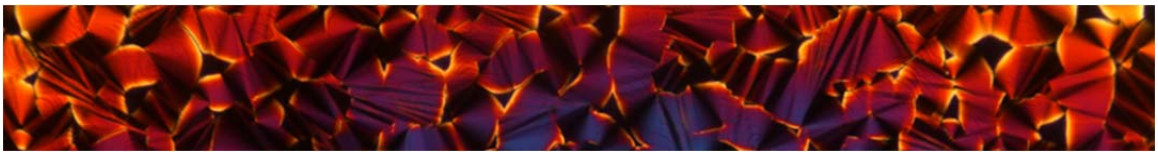

LIQUID CRYSTAL MATERIALS RESEARCH CENTER

SPECIAL SEMINAR SERIES

Self-assembly of Model Microtubules: Shape, Chirality and Twist

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The efficient and controlled assembly of complex structures from macromolecular building blocks is a critical open question in both biological systems and nanoscience. Microtubules are one example of a biopolymer that possesses characteristics quite distinct from standard synthetic polymers that are derived from its monomer being a protein. In order to understand how to design and build artificial polymers that possess features similar to those of microtubules, we have used molecular dynamics simulations to study the self-assembly of model monomers into a tubule geometry. In addition to determining the optimal regime for obtaining tubules, we have calculated a diagram of the structures that form over a wide range of interaction strengths for our model. The self-assembly of free monomers into tubules yields a tubule pitch that often does not match the chirality of the monomer (including achiral monomers). We show that this mismatch occurs because of a twist deformation that brings the lateral interaction sites into alignment when the tubule pitch differs from the monomer chirality. In order to control the tubule pitch by preventing the twist deformation, we employ a lock-and-key interaction and obtain good control of the self-assembled tubule pitch. These results explain some fundamental features of microtubules. The vertical interaction strength is larger than the lateral in microtubules because this yields a better controlled assembly of tubules with the proper pitch. We generally find that the control of the assembly is limited, which explains the range of pitch and protofilament number observed in microtubule assembly.

Wednesday, November 6th at 2:00 p.m. Duane Physics G1B31

Note special time!!

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