

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Brownian dynamics simulation of sickle hemoglobin bundle formation** YA LIU, JAMES GUNTON, Lehigh University, AMIT CHAKRABARTI, Kansas State Univ — The physical properties of biopolymer fibers, such as their stability and degree of aggregation, are implicated in many diseases, including sickle cell anemia. The natural chirality of protofilaments plays a crucial role in the formation of sickle hemoglobin fiber which leads to the permanent blockage of microvessels. We use Brownian dynamics to investigate the kinetics of fiber aggregation. The geometrical helical structure and chirality of the filaments are modeled by anisotropic patch-like interactions. We present the kinetics of fiber formation and study the possibility of a finite critical fiber bundle size. We compare our results with various experimental and theoretical results. This work is supported by grants from the NSF and the G. Harold and Leila Y. Mathers Foundation.

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Date submitted: 18 Nov 2009

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