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Simple Model of Sickle Hemoglobin ANDREY SHIRYAYEV, XIAOFEI LI, JAMES GUNTON — A microscopic model is proposed for the interactions between sickle hemoglobin molecules based on information from the protein data bank. A Monte Carlo simulation of a simplified two patch model is carried out, with the goal of understanding fiber formation. A gradual transition from monomers to one dimensional chains is observed as one varies the density of molecules at fixed temperature, somewhat similar to the transition from monomers to polymer fibers in sickle hemoglobin molecules in solution. An observed competition between chain formation and crystallization for the model is also discussed. The results of the simulation of the equation of state are shown to be in excellent agreement with a theory for a model of globular proteins, for the case of two interacting sites.

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