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Atomistic DMD Simulations of Spontaneous Formation of Nematic and Smectic Phase in a Model Liquid Crystal APICHART LINHANANTA, Lakehead University, IAN MACKAY, University of Guelph — We present atomistic discontinuous molecular dynamics (DMD) simulations of the bulk liquid crystal phases of the molecular fluid 8CB. The model is based on previous DMD models of protein folding (A. Linhananta, J. Boer and Ian MacKay, *J. Chem. Phys.*, 2005, **122**, 114901) in which all atoms including polar hydrogen, but not nonpolar hydrogen, are represented. Bonded pairs interact by infinite square well, while nonbonded atoms interact by hard-sphere square-well potentials. For the model 8CB, molecular parameters are scaled using AMBER and CHARMM force fields. The hard interaction potentials allow very rapid equilibration of ordered phases. Starting the DMD simulations from initial random states, without positional or orientation order, the 8CB systems spontaneously form ordered nematic and smectic phases. The simulations were performed in a 40 A X 40 A X 40 A box with 100 to 500 8CB molecules. At fixed temperature, as the density increases, the phase change from disorder to nematic to smectic. Finally a density-temperature phase diagram is presented.

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