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Adaptive Tempering Monte Carlo Study of Dense Polypyrrole Systems[1] YAFEI DAI, ESTELA BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA 20030 — A modified rigid-ion polarizable model potential of polypyrrole is developed with parameters fitted on multiple points of the electronic energy surface of pyrrole oligomers (n-Py) of different sizes calculated with a hybrid density functional approach [1]. Using this potential, systems containing 192 chains (4-Py) and 64 chains (12-Py) were structurally optimized with the Adaptive Tempering Monte Carlo algorithm [2]. Energetics and structure of these systems were studied as a function of density. Both systems have characteristics of a liquid for densities in the range 0.66 – 1.09 g/cm^3 at T=300 K. The oligomer radius of gyration is insensitive to density changes. However, an orientational order parameter shows a sharp increase as a function of density indicating a tendency of the chains to stack forming regions of aligned chains for the denser systems. [1] Y. Dai, E. Blaisten-Barojas, J. Chem. Phys. 129, 164903(2008); [2] X. Dong, E. Blaisten-Barojas, J. Comp. & Theo. Nanoscience 3, 118 (2006).

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