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Molecular Dynamics Simulations of Polypropylene: Crystallization and Melting[1] MANISH AGARWAL, SHYNO MATHEW, SANAT KUMAR, Columbia University — The crystallization of polypropylene is studied using molecular dynamics (MD), using an all atom force field. Starting from basic ordered arrangements of oligomers, the α and β phases for isotactic polypropylene are recovered, with cell parameters in excellent agreement with crystallographic data. A high pressure phase similar to the smectic phase is also observed. The melting temperatures of these crystals, obtained by isobaric heating, match with the experiments. Oligomers of syndiotactic polypropylene mirror all structural features observed in experiments. The all-trans state is found to be the most stable. The characteristic 2/1 helical structure of syndiotactic polypropylene is also formed along with the all-trans "zigzag" conformation.

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