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Molecular dynamics studies of the structure and dynamics of "perpendicular" layers of *n*-alkane molecules adsorbed on a solid substrate[1] F.Y. HANSEN, Tech. Univ.of Denmark, P. SOZA, P.U. Catolica Chile, H. TAUB, U.Mo.-Columbia, U.G. VOLKMANN, P.U. Catolica Chile — Both AFM and ellipsometry studies of *n*-alkane films adsorbed on a solid substrate from a solution have shown interesting wetting and de-layering phenomena[2]. It was found that on top of one or two "parallel" layers of molecules, where the long axis of the molecules is parallel to the surface, "perpendicular" layers of molecules are formed with the long axis of the molecules perpendicular to the surface. MD simulations of layers of tetracosane, *n*-$C_{24}H_{50,}$ molecules are set up to answer the following questions about the "perpendicular" layers: a) Is the melting transition driven by *gauche* defect creations in the alkane chains like in the parallel layers?, b) can a rotator phase be identified?, c) is there a lateral translational mobility of the chains prior to melting?, and d) what is the mechanism driving the wetting and de-layering transitions in the films? [2]H. Mo et al. Chem. Phys. Lett. **377**, 99 (2003)

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