

Infrared spectroscopic study of the morphology of 3,4,9,10-perylene tetracarboxylic dianhydride films grown on H-passivated Si(111)

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Abstract. Infrared spectroscopy is applied to the characterization of 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) films grown with organic molecular beam deposition (OMBD) on hydrogen-passivated Si(111). Comparing these films with powder spectra, the films show a preferential orientation of the PTCDA molecules close to coplanar with the substrate surface. For deposition of PTCDA films using laser ablation at 1064 nm, the average orientation of the molecules is more random than in the OMBD-grown films, but we still find some degree of preferential order of the molecules with respect to the substrate surface. The experimental findings are compared to density functional calculations of the single molecule and the two crystalline phases.

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