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Evidence for strong interaction of PTCDA molecules with defects on sulphur-passivated GaAs(100)

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Abstract
Raman spectroscopy was employed to investigate the initial stage of interface formation between 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) molecules and sulphur-passivated GaAs(100) surfaces. Monitoring the Raman spectra for submonolayer coverage as well as after annealing above the desorption temperature of PTCDA reveals the presence of a C- H mode which is shifted by 13 cm^{-1} towards lower frequency compared to its value in bulk PTCDA. The molecules remaining at the surface after annealing are proposed to interact with surface defects predominantly induced by the dopant atoms. This proposal is supported by density-functional theory calculations considering the interaction of dopant atoms with single molecules.

PACS
68.60.-p - Physical properties of thin films, nonelectronic.
68.35.Dv - Composition, segregation; defects and impurities.
78.30.Jw - Organic compounds, polymers.