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Oxygen and water defect formation processes in pentacene. LEONIDAS TSETSERIS, SOKRATES PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — Organic thin-film devices have emerged as promising candidates for novel electronic applications. Unlike traditional solid-state devices, the weak intermolecular non-covalent bonding of organic thin films leads to flexibility and possible pattern formation. The same mechanism, however, is responsible for the appearance of a variety of defects that may interfere with film growth and are potentially detrimental to the desired transport properties. Here we use first-principles calculations to study defect formation processes in the prototypical system of pentacene. In particular, we report on defect configurations of oxygen and water molecules in bulk pentacene and ultra-thin films on Si-based substrates. The results show that several stable configurations of such defects exist. Their presence has a direct bearing on growth processes and transport properties through strong covalent bonding and induced molecular distortions in their vicinity. This work was supported in part by DOE Grant DEFG0203ER46096.

Leonidas Tsetseris
Vanderbilt University

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