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Vacancy effects on the electronic and structural properties pentacene IFLAH LARAIB, ANDERSON JANOTTI, Univ of Delaware — Defects in organic crystals are likely to affect charge transport in organic electronic devices. Vacancies can create lattice distortions and modify electronic states associated with the molecules in its surrounding. Spectroscopy experiments indicate that molecular vacancies trap charge carriers. Experimental characterization of individual defects is challenging and unambiguous. Here we use density functional calculations including van der Waals interactions in a supercell approach to study the single vacancy in pentacene, a prototype organic semiconductor. We determine formation energies, local lattice relaxations, and discuss how vacancies locally distort the lattice and affect the electronic properties of the host organic semiconductor.

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