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First principles study of defects in nanotubes JESSICA GALLAGHER, ETHAN MINOT, GUENTER SCHNEIDER, DAVID ROUNDY, Oregon State University — Engineered defects in carbon nanotubes (CNTs) have proven useful in electrical device applications such as self-assembled CNT circuits, gas sensors and single molecule sensors. In many cases the nature of the defects is largely unknown. We present an *ab initio* study investigating the effects of several varieties of defects on the electronic structure of single walled carbon nanotubes. The defects studied include the single-carbon vacancy, a single-carbon vacancy passivated with hydrogen, and a single sp^3-bonded carbon. Within the framework of density-functional theory in the local density approximation, we have investigated the effect of these vacancies and other defects on the local band gap and speculate as to their effects as scattering centers.

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