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Re-entrant semiconducting behavior of zigzag carbon nanotubes on substitutional doping by oxygen dimers SEUNG-HOON JHI, Department of Physics, POSTECH — The electronic structures of carbon nanotubes doped with oxygen dimers are studied using the *ab initio* pseudopotential density functional method. The fundamental energy gap of zigzag semiconducting nanotubes exhibits a strong dependence on both the concentration and configuration of oxygen dimer defects that substitute for carbon atoms in the tubes and on the tube chiral index. For a certain type of zigzag nanotube when doped with oxygen dimers, the energy gap is closed and the tube becomes semimetallic. At higher oxygen-dimer concentrations the gap reopens, and the tube exhibits semiconducting behavior again. The change of the band gap of the zigzag tube is understood in terms of their response to the strains caused by the dimer substitutional doping.

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