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The structural and electronic properties of vacancy clusters in carbon nanotubes ALEX TAEKYUNG LEE, YONG-JU KANG, KEE JOO CHANG, Korea Advanced Institute of Science and Technology — Carbon vacancies, which can be generated by electron or ion irradiation, significantly modify the structural and electronic properties of carbon nanotubes. Recent experiments showed that vacancy-type defects induce structural changes such as junction, shrinkage, and bending. In this work we study the atomic and electronic structure of vacancy clusters up to six missing atoms in carbon nanotubes through both first-principles and tight-binding calculations. We find that vacancy defects are generally stable when they are aligned along the tube axis, forming a vacancy-chain. Due to the curvature effect, this feature is different from that found for graphene, where vacancies tend to aggregate into a lump. For the even-numbered vacancies in the (5,5) and (9,0) nanotubes, we find that clustering of vacancies leads to the local shrinkage, with a smaller diameter tube sandwiched between two semi-infinite tubes. In this case, the defect levels near the Fermi level are mostly associated with 7- or 8-membered rings, whereas those for odd-numbered vacancies result from the remnant dangling bonds.

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