Lee *et al.* Reply: In Ref. [1], we reported our experimental observation of two different types of paired gap states, deep and shallow levels, in a semiconducting carbon nanotube (CNT). With a first-principles study, we interpreted that the former originates from vacancy-adatom (VA) complex, while the latter comes from a topological defect such as a pentagon-heptagon (PH) structure [1,2]. In the preceding Comment [3], Krasheninnikov, Foster, and Nieminen offer an alternative explanation that the paired gap states may stem from two close single atom defects, such as hydrogen adatoms or vacancies. Here we argue that two close defects consisting of hydrogen adatoms or vacancies do not match our experimental data.

First, they claimed that the formation energy of VA and PH structures may be too high for the reaction to take place. The PH structures in our report are not confined to Stone-Wales ($5-7-7-5$) defects. They may have various configurations with five- and seven-membered rings in a hexagonal network. Such structures have been observed before [4,5], and we do not think the issue of abundance is essential. In the Stone-Wales transformation, the activation energy barrier was estimated earlier as 5–6 eV, but recent studies discovered that it can be reduced considerably by autocatalysis reactions [6,7]. These structures have intensively been studied by many theory groups, because their activation energy barrier is accepted as reasonably low, compared to other reaction pathways. We suspect that the dissociation energy barrier of a hydrogen molecule must be even higher than that of the transformation with autocatalysis. (By the way, the estimated defect density they mentioned was originally in a theory paper [8], rather than in an experiment paper [9].)

Second, they claimed that the recombination energy of VA and PH structures may not be high enough, considering the annealing temperature of $\sim 150\,^{\circ}\mathrm{C}$. For the recombination, the rebonded C-C bond (1.57 Å) must be broken in advance. Since the bonding energy of a single C-C bond is ~ 3.5 eV, such a reaction is unlikely. After the annealing process, however, a C atom may form a VA defect. In addition, the recombination energy they assumed to estimate the lifetime (~ 1 eV) seems too low. If the activation energy barrier height is 1.7 eV, the lifetime of a defect becomes several years due to the exponential factor.

When two hydrogen adatoms approach each other, they can produce paired states whose energy splitting depends on coupling strength or spatial separation. Since a hydrogen adatom produces a half-filled localized state pinned at the Fermi level, one of the paired states should be an occupied state, while the other being an unoccupied state. In our experimental observation, however, both deep levels are unoccupied, located above the Fermi level. Even if electron transfer from the CNT to the gold substrate is considered, there exists a first-principles calculation including the gold substrate which reports that the originally highest occupied state is not empty [10]. For shallow levels, the spatial distance between them is estimated to be ~ 1 nm from the maximum peak positions of our experimental data, and the energy splitting is ~ 0.5 eV. According to our calculation, such an energy splitting can be made when a hydrogen adatom is the nearest neighbor or next nearest neighbor to the other hydrogen atom. Then the distance between them will be ~ 0.25 nm, which is much shorter than the experimental observation. Our arguments are applicable to two close vacancies as well.

In conclusion, our VA and PA models are simple local structures which exhibit major features of our experimental observations. Although two hydrogen adatoms or vacancies in vicinity may give rise to two levels, they do not agree with our experimental observation.

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