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Ab initio* investigations of formation of the poly-bromine anions encapsulated inside the carbon nanotube.** DONGCHUL SUNG, Sejong University, Seoul, Korea, NOEJUNG PARK, Dankook University, Seoul, Korea, SUKLYUN HONG, Sejong University, Seoul, Korea — We have performed ***ab initio density-functional calculations to investigate the electronic and geometric structure of the bromine adsorbates inside the carbon nanotube. It is found that the charged odd-membered molecular species (Br_3 or Br_5) are energetically favored inside the carbon nanotube rather than common Br_2 molecule. Vapor phase of bromine molecules (Br_2) could exothermically adsorb into the nanotubes, and in turn, transform into the Br_3 or Br_5 structures without a significant energy barrier. Such a formation of the poly-bromine anions accompanies a strong charge transfer from the nanotube to the adsorbates, rendering the encapsulating nanotube strongly hole-doped. We suggest that an exposure of the tip-opened carbon nanotube samples to a modest Br_2partial pressure could result in strong hole-doped, and thus nearly metallic nanotube samples.

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