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Electronic properties of Aluminum Doped Carbon Nanotubes with Stone Wales Defects: Density Functional Theory *

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Al-doped single wall carbon nanotube with Stone Wales defect was theoretically analyzed, two different orientations of chiral $(8,4)$ carbon nanotubes was doped among the joints of defective carbon rings. Density functional theory was implemented to study structural and electronic properties of Al-doped chiral carbon nanotubes. Doping bond lengths as well as their geometrical structure were determined at the different orientations. The electronic properties were also illustrated by evaluation band of the gap energies at each possible doping site. Our results indicated that not only Al-doping tune the band structure, but also dopant site played a crucial rule on manipulating physical properties of chiral carbon nanotubes.

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