

Abstract Submitted
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Electronic Property Control of Single-Walled Carbon Nanotubes by Functionalization CHIAYUN WU, YOUNG-KYUN KWON, Univ of Mass - Lowell — Single-walled carbon nanotubes exhibit remarkable electronic properties. It is well known that there are two types of single-walled carbon nanotubes: metallic and semiconducting. However, separating semiconducting carbon nanotubes from metallic ones is a “holy grail” problem in nanoelectronics fields. Using ab initio density functional theory, we will present the effects of various functional groups, such as 4-bromobenzene diazonium tetrafluoroborate, on SWNTs. Modifications in electronic and transport properties due to such functionalization will be discussed. Possible mechanism converting metallic tubes to semiconducting ones will be addressed.

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