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Effect of Localized Covalently Attached Oxygen Functionalization on the Transport Properties of Metallic Carbon Nanotubes MD. ASHRAF, Univ. of Califonia Riverside, NICOLAS BRUQUE, Univ. of California, Riverside, RAJEEV PANDEY, Univ. of the Pacific, PHILIP COLLINS, Univ. of California Irvine, ROGER LAKE, Univ. of California Riverside — We perform of a comprehensive study of the effect of covalent oxygen attachment on the transmission of metallic carbon nanotubes (CNTs). Oxygen attachment on the CNT surface favors an ether type bond. Two oxygen atoms attached on the CNT surface within the same carbon ring on parallel bonds are energetically the most stable attachment configuration. In an armchair CNT, oxygen attachment favors the C-C bonds orthogonal to the CNT axis. Correlated addition propagates axially along parallel orthogonal bonds. In a zigzag CNT, oxygen attachment prefers the slanted bond, and correlated addition propagates spirally along parallel slanted bonds. Closely spaced oxygen attachment on the armchair and zigzag CNT surfaces causes a dip in transmission symmetrically away from the Fermi level. A clustered group of oxygen atoms covalently attached to a single-walled metallic zigzag CNT can result in a one order of magnitude drop in transmission that is asymmetric with respect to the Fermi energy resulting in a qualitative resemblance to conductance versus gate voltage curves observed experimentally [Science 315, 77 (2007)]. Calculations use density functional theory combined with non-equilibrium Green functions.

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