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Theoretical Study of Side Wall Ozonation of Single-Wall Carbon Nanotubes BRAHIM AKDIM, Air Force Research Lab, XIAOFENG DUAN, Air Force Research Lab, TAPAS KAR, Utah State University, RUTH PACHTER, Air Force Research Lab — Oxidation of single-wall carbon nanotubes (SWCNTs) by ozone has been utilized extensively, for example, in the elimination of amorphous carbon in purification processes, for opening closed tips and sidewalls of nanotubes to maximize the rate of metal adsorption and hydrogen uptake, as well as to facilitate functionalization for achieving solubility. In this work, we present a density functional theory study, to investigate the adsorption mechanisms of O_3 on the sidewall of metallic C(5,5), and semiconducting C(10,0) SWCNTs, in the presence and absence of Stone-Wales defects with different morphologies. The energetics, electronic structures, and Raman modes shifts, upon adsorption, as compared to pristine tubes, will be discussed in detail.

Prefer Oral Session
 Prefer Poster Session

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