

Abstract Submitted
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Effects of the Modification of Single- and Double-Wall Carbon Nanotubes: A Theoretical Study of Field Emission Properties BRAHIM AKDIM, Air Force Research Lab, TAPAS KAR, Utah State University, XIAOFENG DUAN, ASC/MSRC, RUTH PACHTER, Air Force Research Lab — In this work, we report first principles calculations of modified single-wall carbon nanotubes (SWCNTs) by O_3 and $-COOH$ functionalization, as well as of double-wall carbon nanotubes (DWCNTs) by Cs surface adsorption. Properties related to field emission, including the effects of an applied electric field to mimic the emission environment, as well as structural parameters, are discussed. The results, which suggest a suppression of the emission upon ozone adsorption and carboxy-functionalization in SWCNTs, but an enhancement with Cs surface adsorption, are explained in detail. Finally, the effects of treating DWCNTs with Cs adsorption, as compared to our previous results for SWCNTs, are summarized.

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