

Abstract Submitted  
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**All About Chlorinated Carbon Nanotubes<sup>1</sup>** DOGAN ERBAHAR, SAVAS BERBER, Gebze Institute of Technology — The halogens are viable alternatives to harsher chemicals in the post-process of purification of carbon nanotube production. However the chlorine is known to bind less aggressively to carbon nanotubes than fluorine and hydrogen. Therefore, in principle the residual Cl left after the halogen gas treatment of the nanotubes can be removed without damaging the nanotube walls easier. We report ab initio density functional calculation results about pure and defective carbon nanotubes of various diameters interacting with single and multiple chlorine atoms. We first focus on pure nanotubes and investigate the adsorption of additional Cl atoms near the first adsorption site, investigate the clustering tendency and most favourable configurations. We report the energetics results as well as the alteration of electronic properties. We then focus on monovacancy and divacancy defects on carbon nanotubes. It is a known fact that the defective site to be more active in this case. We apply the same procedure as in the pure nanotubes but also investigate the effect of chlorination on reconstruction process and also electronic transport properties.

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