Abstract Submitted
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The chlorination of carbon nanotubes[1] DOGAN ERBAHAR, SAVAS BERBER, Gebze Institute of Technology — We use *ab initio* density functional calculations to study the chlorination of pure and defective carbon nanotubes. We first focus on the adsorption of a second Cl after the adsorption of the first Cl atom. We find that the second Cl prefers to adsorb closer to the first adsorption site. We then search for the clustering tendency of the adsorbates, and determine the optimum adsorption configurations for different Cl coverages. Unlike for adsorption outside the nanotube, the adsorption inside the nanotube is only physisorption, and the atomic structure is governed by the charge transfer. We observe that the chemisorption is energetically more favorable in small diameters while the energy difference for large diameters is not significant. Therefore, the residual Cl left after the halogen gas treatment of the nanotubes can be removed without damaging the nanotube walls. Note that the halogens are viable alternatives to harsher chemicals in the purification. However, we find that the Cl atoms adsorb on defects more strongly, and the adsorbates may initiate significant structural reconstructions of the defects. Last, we obtained activation energies during the adsorption of a Cl pair on a carbon nanotube.

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