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$AuCl_4$ Functionalized Carbon Nanotubes: Origin of the p-Type Doping ALTYNBEK MURAT, PSE Division, KAUST, Saudi Arabia, IVAN RUNGGER, STEFANO SANVITO, School of Physics, AMBER and CRANN Institute, Trinity College, Dublin 2, Ireland, UDO SCHWINGENSCHLÖGL, PSE Division, KAUST, Saudi Arabia — The microscopic origin of the p-type doping of $AuCl_3$ functionalized carbon nanotubes (CNTs) is investigated using first-principles self-interaction corrected density functional theory. Although the system has been studied as potential candidate for highly sensitive and selective gas sensors, a clear identification of the source of the p-type doping is not achieved. Recent experimental and theoretical works suggest that it is due to the adsorbed Cl atoms. We test this hypothesis and show that adsorbed Cl atoms only lead to a p-type character for very specific concentrations and arrangements, which furthermore are not the lowest energy configurations. We therefore propose and investigate alternative mechanisms while considering all possible configurations and concentrations. In particular, we study the possible formation of different conformations of $AuCl_3$ as well as the effect of the adsorbate concentration. As a result, we find that especially $AuCl_4$ molecules bind strongly to the CNT and that they lead to an electron transfer to the molecules and thus a shift of the Fermi energy below the valence band maximum. We conclude that the origin of the p-type doping in $AuCl_3$ functionalized CNT is due to the adsorption of $AuCl_4$ molecules.

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