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Reactivity of silicon and germanium doped CNTs toward aromatic sulfur compounds: A theoretical approach

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Abstract

Adsorption processes of thiophene and benzothiophene on pristine carbon nanotubes (CNTs), and on CNTs doped with Si or Ge, have been modeled with Density Functional. This is the first study on the chemical reactivity of such doped tubes. The calculated data suggest that the presence of silicon or germanium atoms in CNTs increases their reactivity toward thiophene, and benzothiophene. The adsorption of these species on pristine CNTs seems very unlikely to occur, while the addition products involving doped CNTs were found to be very stable, with respect to the isolated reactants, in terms of Gibbs free energy. Several of these adsorption processes were found to be significantly exergonic ($\Delta G < 0$) in non-polar liquid phase. The results reported in this work suggest that Si and Ge defects on CNTs increase their reactivity toward unsaturated species, and could make them useful in the removal processes of aromatic sulfur compounds from oil-hydrocarbons. However, according to our results, CNTs doped with Si atoms are expected to be more efficient as aromatic sulfur compounds scavengers than those doped with Ge. These results also suggest that the presence of silicon and germanium atoms in the CNTs structures enhances their reactivity toward nucleophilic molecules, compared to pristine carbon nanotubes.

Keywords: Adsorption; Carbon nanotubes; Thiophene; Benzothiophene; Silicon; Germanium