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First principles study of NH₃ adsorption on carbon nanowires
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Corrosion (UACAM) — Recently has been reported a new type of one-dimensional
carbon structures. Carbon nanowires formed by a linear carbon-atom chain in-
side an armchair (5,5) carbon nanotube has been observed using high-resolution
transmission electron microscopy. Theoretical and experimental studies of the NH₃
adsorption in the carbon nanotubes report changes in the electronic properties of the
carbon nanotubes. In the present work we have studied the electronic and structure
properties of carbon nanowires (chain@SWCNT) when NH₃ atoms are adsorbed.
We used the Density Functional Theory and the calculations were performed by
the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient
Approximation (GGA) for the exchange-correlation potential. We have analyzed
the changes in the atomic structure and density of states (DOS). We found that
the electronic character of the carbon chain of the chain@SWCNT system, can be
modulate by NH₃ adsorption. This research was supported by SEP under Grant
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