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Determination of the vibration frequencies of Carbon Nanotubes and Carbon Nanoribbons[1] M. PACHECO, Universidad Federico Santa Maria, A. LEON, Universidad Diego Portales — The optical properties of organic materials are similar to the properties of the molecules that constitute it. This motivates the study of molecular complexes that would form new materials. Interesting optical properties are observed in conjugated polymers due to delocalized π electrons, which allow transitions in the visible spectrum. In this work we present results of the vibration spectrum for pristine and functionalized carbon nanoclusters. The electronic properties are obtained by first principles calculations, based on the Becke-Perdew GGA approximation. The frequencies are computed numerically by differentiation of the energy gradients in slightly displaced geometries. The three stages of calculations will be performed using the ADF code. The geometric optimization protocols for pristine and functionalized structures are made adopting the "quasi Newton approach." The vibration spectra show interesting properties when the structures are functionalized with organic molecules.

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