Poster

Electron excitations of carbon nanostructures by the CNDOL Hamiltonian

A.L. Montero[a,b] , M.E. Fuentes[c], E. Menéndez[d], W. Orellana[e], C. Bunge[f], L.A. Montero[a] and J.M. García de la Vega[b]

a) Laboratorio de Química Computacional y Teórica, Facultad de Química, Universidad de la Habana, 10400 Havana, Cuba
b) Departamento de Química Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid, 28049 Madrid, Spain
c) Laboratorio de Química Computacional, Universidad Autónoma de Chihuahua, 31000 Chihuahua, Mexico
d) Departamento de Física, Facultad de Ciencias, Universidad de Chile, Las Palmeras 3425, 780-0024 Ñuñoa, Santiago, Chile
e) Departamento de Ciencias Físicas, Universidad Andrés Bello, Av. República 220, 837-0134 Santiago, Chile
f) Instituto de Física, Universidad Nacional Autónoma de México, México
ana.montero@uam.es

Real scenarios at nanoscopic levels involve irreducible large molecular systems that are characterized by complex environments and non-periodic arrangements of different bodies. Consideration of electron densities and exchange by means of appropriate Hamiltonians of the complete system is required to obtain more reliable computational models, including bonding. Electronic state properties of such systems, like fullerenes [1] and nanotubes [2], represent a very active field of research nowadays where, for example, the interaction with the light is important.

CNDOL (Complete Neglect of Differential Overlap considering the L azimuthal quantum number), is an *a priori* and approximate quantum mechanical Hamiltonian [3] that consists in a simplified Hartree-Fock (HF) procedure comprising all valence electrons. It is provided as a good starting point to build molecular wave functions, which are further variationally improved by applying large-scale singly-excited configuration interaction (CIS) as a straightforward procedure for modeling electron excitation processes of big polyatomic systems[4].

In the present work we want to show the performance of the CNDOL formalism to model the electronic properties of different carbon nanostructures. The predicted electron transition energies and related properties of the isolated fullerene (C_{60}), van der Waals cluster models of them $(C_{60})_n$ and zig-zag like (n,0) single walled carbon nanotubes (SWCNT), are analyzed and compared with available experimental data. The optical spectrum of the isolated fullerene and their cluster models show similarities. However, the appearance of allowed electron transitions at lower energies in van der Waals complexes in concordance with the experimental spectra, could be considered as an evidence of intermolecular interaction phenomena during excitations. The CNDOL calculations of (5,0), (9,0) and (13,0) SWCNT´s, performed over a set of increasingly long, although finite lengths, show that it is

important to consider finite models of SWCNT's with length larger than 3 nm in order to simulate realistic properties corresponding to experimental systems. The absorption spectrum obtained for (5,0) SWCNT is in nice agreement with the experimental data [5]. Both, the (5,0) and (13,0) SWCNTs do not show a decrease in the lowest energy excited states when the length increases, in contrast to the (9,0) SWCNT, which show more favoured conditions for photo-excitations when became longer.

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