BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA

INSTITUTO DE FÍSICA
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SEMINARIO EXTRAORDINARIO
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"Lattice dynamics and electron-phonon coupling in carbon nanotubes"

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Lattice dynamics of small radius nanotubes has received a lot of attention due to the competition between superconductivity and Peierls /Charge density wave order. So far all ab-initio calculations for isolated nanotubes with diameter of 4A have shown a strong tendency to either a Peierls transition ((in (3,3)-tubes) [1] or a structural transition to a non-metallic state with a small gap ((5,0)-tubes) [2] in contrast to experimental findings in 4 A tubes [3]. Doping these tubes might offer a possibility to enhance superconductivity , an effect which is well known from intercalated graphite. Ab-initio calculations of the lattice dynamics and electron-phonon coupling for doped (3,3)-tubes show an increase of the transition temperature to the superconducting state, however in isolated tubes the Peierls transition is still favored. We have also studied these effects in coupled nanotube arrays (nanotube bundles) . Using density functional theory and density functional perturbation theory we have investigated the lattice dynamics and electron-phonon coupling for (3,3) –tubes as function of the intertube coupling. Charge density wave order is strongly coupling dependent leading to favoring eventually the superconducting state. Comparison with available experimental information will be presented.

[1] K.-P. Bohnen, R. Heid ,H. J .Liu ,C. T. Chan , PRL 93, 245501 (2004)
[2] D. Connetable et al. , PRL 94, 015503 (2005)
[3] Z .K. Tang et al. , Science 292, 2462 (2001).

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