POSTER

NANOTUBES' BAND THEORY

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INTRODUCTION

We propose overlap integrals and band theory calculations for two particular nanotubes using a theoretical calculation derived from the well known Wallace's graphite tight-binding model for graphite.

CRYSTAL POTENTIAL

The crystal potential used for nanotubes in the frame of our band calculation is validated by reduction to a graphitic plane potential. We neglect the specific term associated to the cylindric shape of the nanotubes.

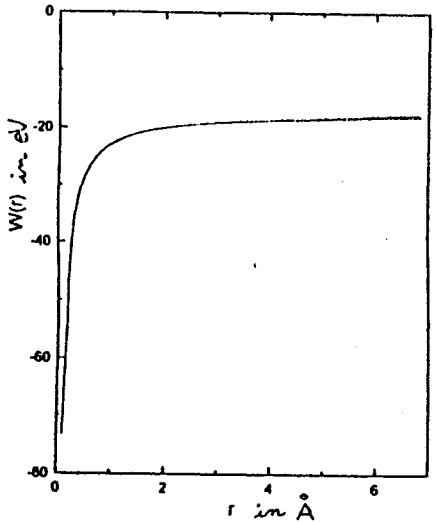

Figure 1 Crystal potential

This spherical potential is given in table 1 and shown in figure 1 as a function of the distance r.

Table 1 Crystal potential

r	$W(r)$	r	$W(r)$	r	$W(r)$
0.1	−73.313	0.2	−45.255	0.3	−35.897
0.4	−31.216	0.5	−28.407	0.6	−26.535
0.7	−25.197	0.8	−24.194	0.9	−23.413
1.0	−22.789	1.1	−22.278	1.2	−21.852
1.3	−21.492	1.4	−21.183	1.5	−20.916
1.6	−20.682	1.7	−20.475	1.8	−20.292
1.9	−20.127	2.0	−19.979	2.1	−19.846
2.2	−19.724	2.3	−19.613	2.4	−19.511
2.5	−19.417	2.6	−19.331	2.7	−19.251
2.8	−19.177	2.9	−19.107	3.0	−19.043
3.1	−18.982	3.2	−18.926	3.3	−18.872
3.4	−18.822	3.5	−18.775	3.6	−18.731
3.7	−18.688	3.8	−18.648	3.9	−18.610
4.0	−18.574	4.1	−18.540	4.2	−18.508
4.3	−18.476	4.4	−18.447	4.5	−18.418
4.6	−18.391	4.7	−18.365	4.8	−18.340
4.9	−18.316	5.0	−18.293	5.1	−18.271
5.2	−18.250	5.3	−18.230	5.4	−18.210
5.5	−18.191	5.6	−18.173	5.7	−18.155
5.8	−18.138	5.9	−18.122	6.0	−18.106
6.1	−18.091	6.2	−18.076	6.3	−18.062
6.4	−18.048	6.5	−18.034	6.6	−18.021
6.7	−18.008	6.8	−17.996	6.9	−17.984

The Slonczewski-Weiss parameters [1] computed, making use of our crystal potential show good values: see table 2 for a comparison of theoretical and experimental values [2][3].

Table 2 SW parameters

param.	*theoretical*	*experimental*[4]
γ_0	2.8	$2.8 \prec \gamma_0 \prec 3.2$
γ_1	0.39	$0.27 \prec \gamma_1 \prec 0.40$
γ_2	0.00023	$0.018 \prec \gamma_2 \prec 0.02$
γ_3	0.2	$0.14 \prec \gamma_3 \prec 0.29$
γ_4	0.2	$0.2 \prec \gamma_4 \prec 0.3$
γ_5	0.00023	$0.018 \prec \gamma_5 \prec 0.02$
γ'	-0.41	?

Our potential associated to a Wallace's tight binding model [5] enables numerical computations of matrix elements in the secular determinant with a Slater's wave functions basis and leads to null values for $(2S,2P_x,2P_y)$ and $2P_z$ interaction terms as expected. Our results prove $\pi$and σ band separation for a graphene sheet. We also verify a 20 eV [6] width for the $\Gamma_{2g}^- - \Gamma_{2u}^-$ transition along K-Γ symmetry line in the Brillouin zone (this is shown in figure 2).

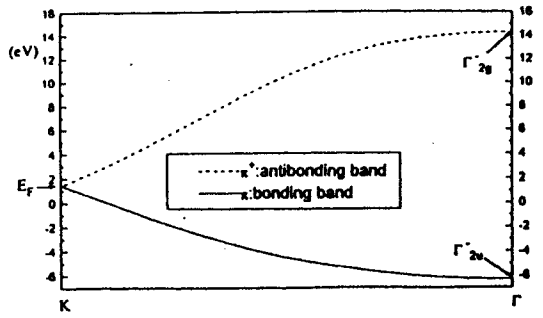

Figure 2 Energy bands

These results confirm the realistic feature of our potential in its total form when applied to nanotubes.

CONCLUSIONS

The Hamiltonian elements evaluation in a new basis set of atomic orbitals ($2S'$, $2P'_x$,$2P'_y$, $2P'_z$) for nanotubes need introduction of a warped potential term. Under these conditions overlap and potential integrals are no longer zero for ($2S'$,$2P'_x$,$2P'_y$) and $2P'_z$ interactions: σ and π bands interact. This is in accordance with Coulson's [7] group theoretical predictions for non-planar compounds. Electronic and mechanical properties of nanotubes are related to this band theoretical calculations (see the contribution in the same session entitled Resistivity of Samples Containing Nanotubes).

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