Current induced forces on adsorbates at conducting carbon nanotubes

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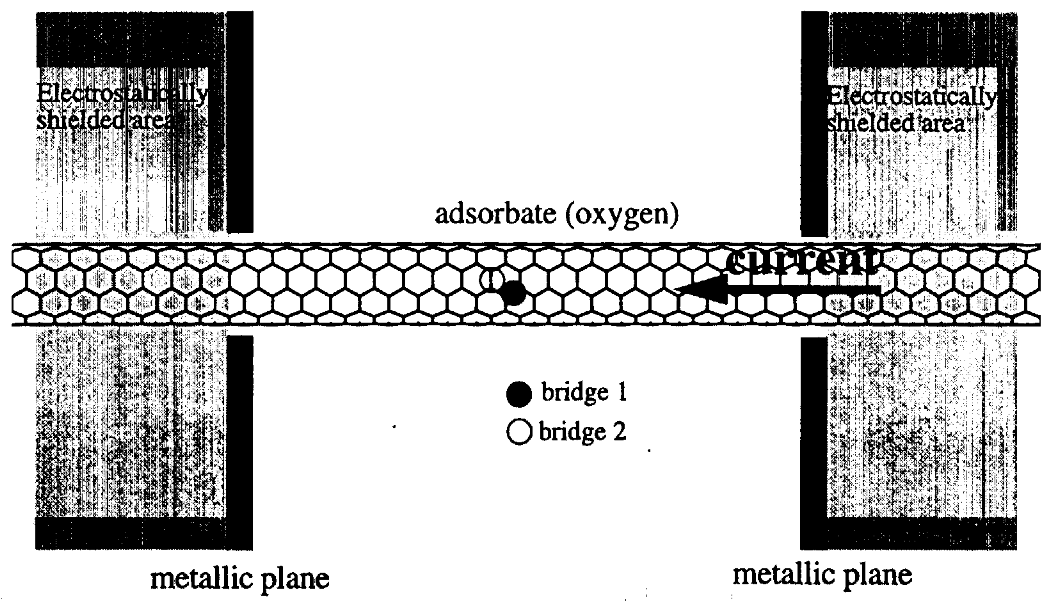
1. Statement of the problem

Force on an impurity due to electric current.
Fact: high current density available
-> How big is the force? What is its direction? How does it depend on the voltage?

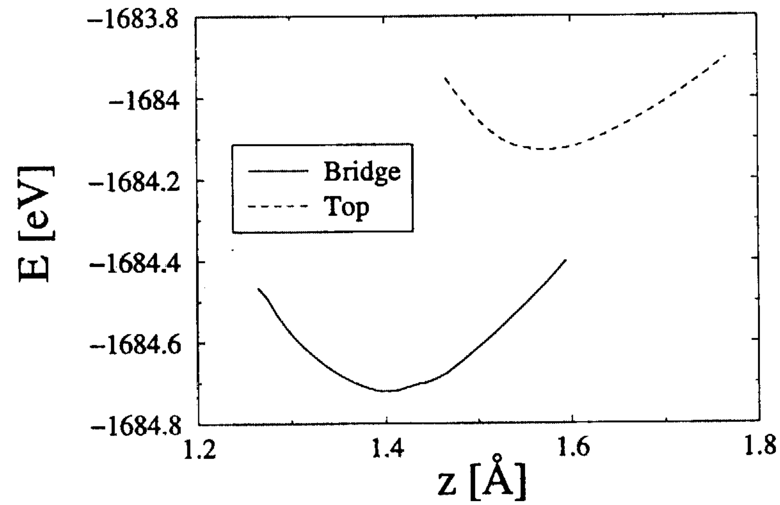


2. Implementation:
First principles LCAO + Green's Function approach

Ab initio Hamiltonian
for equilibrium

from "fireball" [1,2]
(non-orthogonal)

Lowdin transformation
to orthogonalise



Self-consistent
non-equilibrium Green
function

-> charges and forces

Theory of current induced mean forces [2,3]

(1) $$F_\alpha \equiv \frac{d}{d\alpha}E = \sum_{ij} \delta q_{ij} \frac{dH_{ij}}{d\alpha} \quad ,$$

(2) $$q_{ij} = \int_{-\infty}^{\infty} f(E) \rho_{ij}^{tot}(E)dE + \int_{-\infty}^{\infty} [f(E-eV) - f(E)] \rho_{ij}^{trans}(E)dE$$

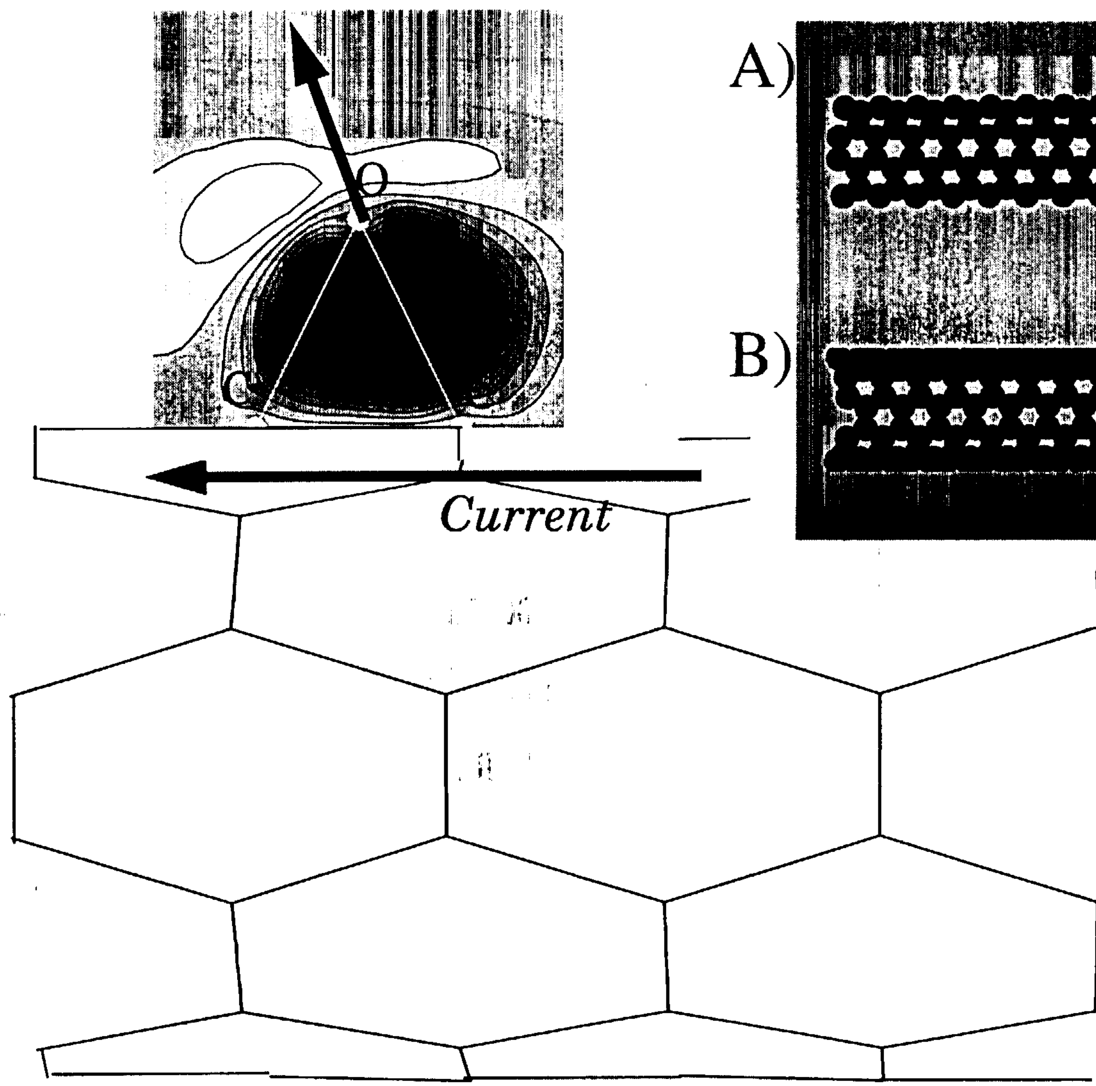
[1] Demkov, A.A.; Ortega, J.; Sankey, O.F.; Grumbach, M.P. Phys. Rev. B , 52, 1618 (1995); O.F.Sankey and D.J.Niklewski, Phys.Rev.B 40, 3979 (1989).

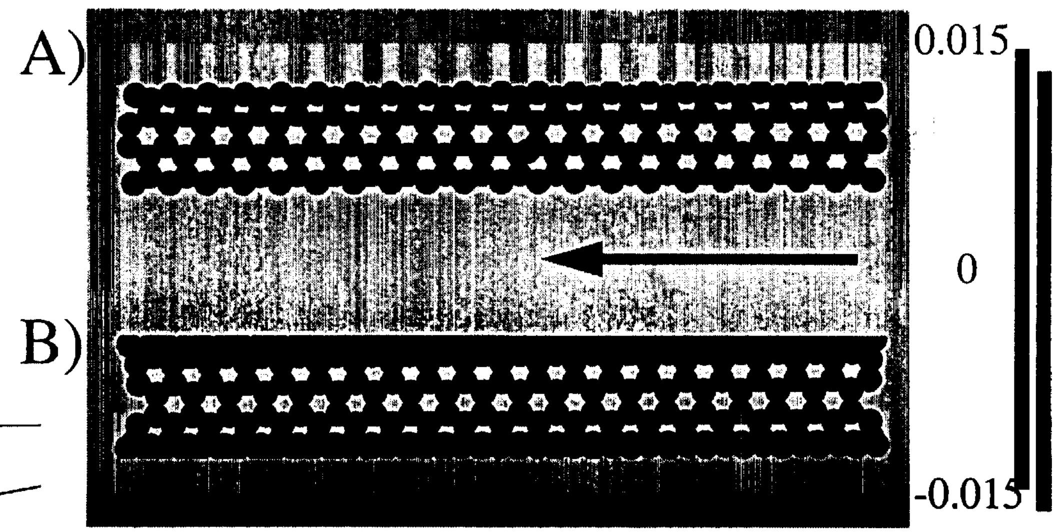
[2]T.N.Todorov, J.Hoekstra and A.P.Sutton, Philos.Mag.B 2000, vol80, no.3, 421.

[3] N.Mingo, Liu Yang and Jie Han, submitted.

3. Results

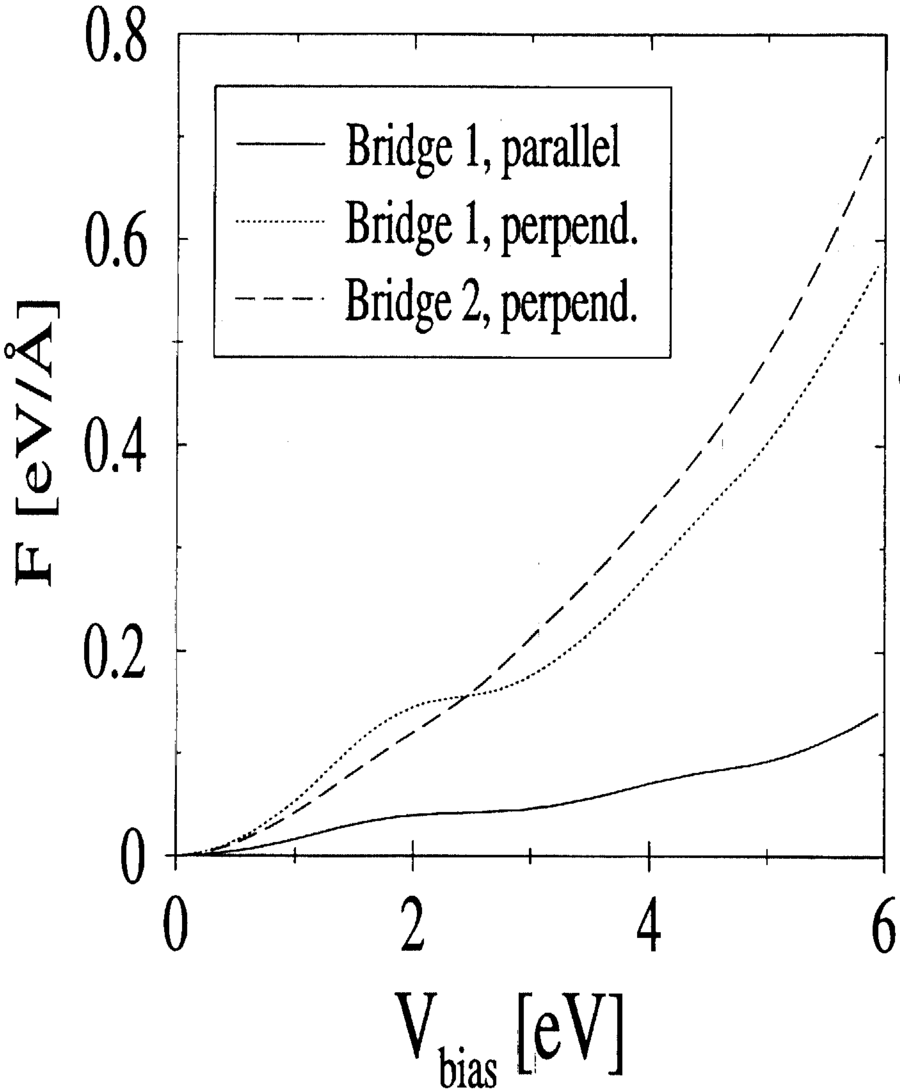
3.1. Non-equilibrium charge density

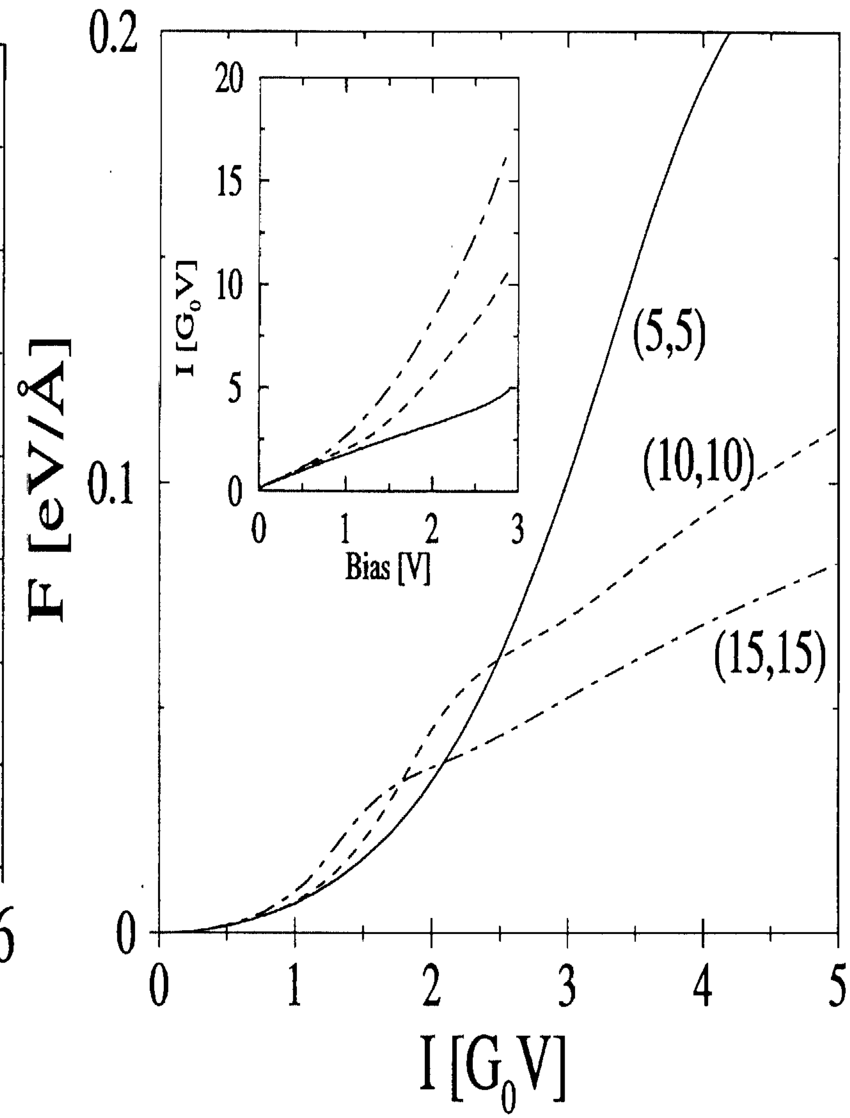


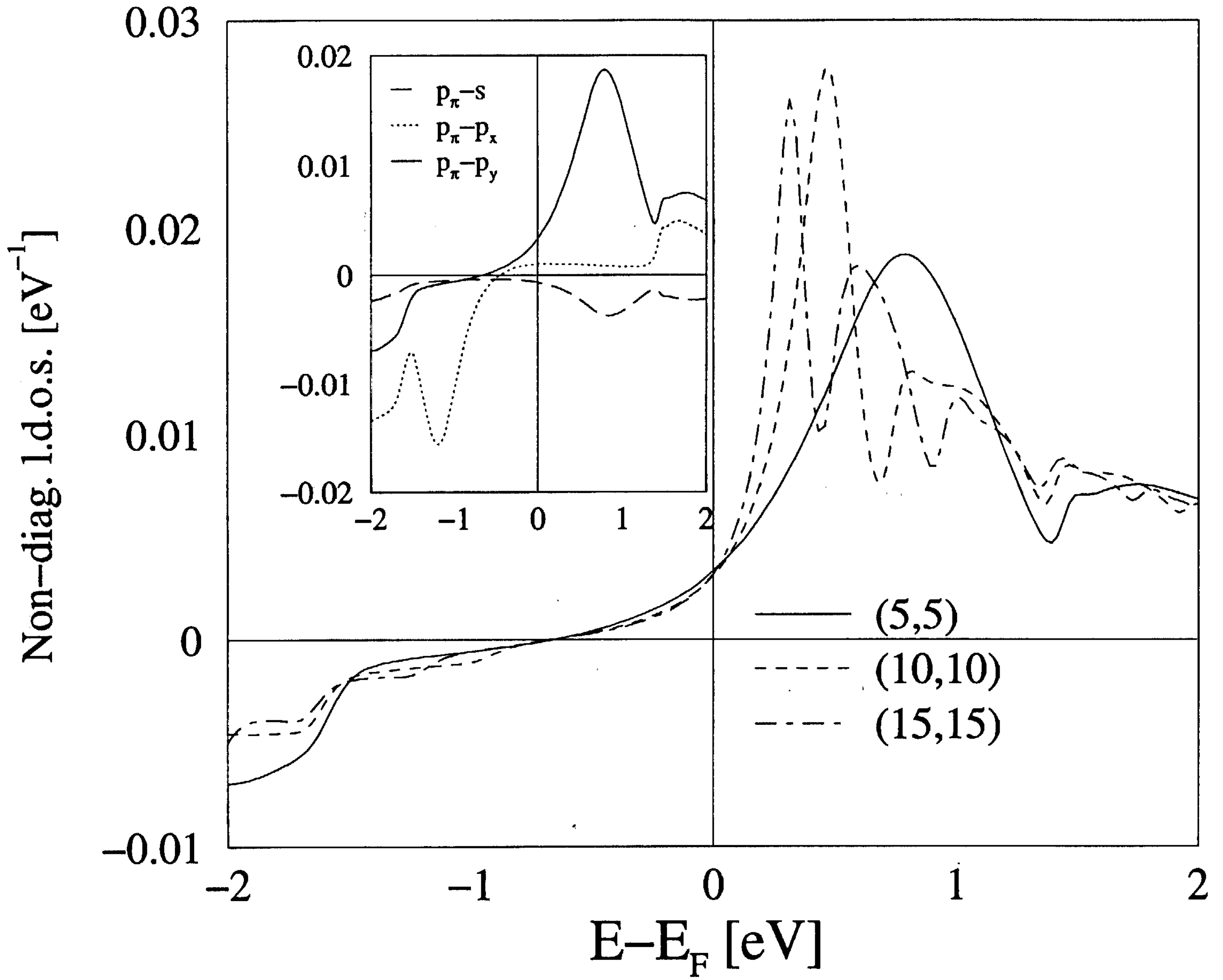


1V

3.2. Induced force







0.03
0.02
0.01
0
−0.01
−2
−1
0
1
2
Non−diag. l.d.o.s. [eV^{-1}]
E−E$_F$ [eV]
(5,5)
(10,10)
(15,15)
p_π−s
p_π−p_x
p_π−p_y

4. Conclusions

Induced mean force (O on armchair):

-> Directed outwards + a smaller component in the electron flow direction.

-> ~0.7eV for a 6V bias pulse -(5,5)-. Enables induced diffusion.

-> At low bias, force is larger for larger radius, and crosses over to the opposite trend when increasing the bias. The crossover current is approximately inversely proportional to the radius, $I_c \sim 1.5/n\ VG_0$.