UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA

Theoretical spectroscopy characterization of deep electronic states due to implanted Ge atoms in Silicon

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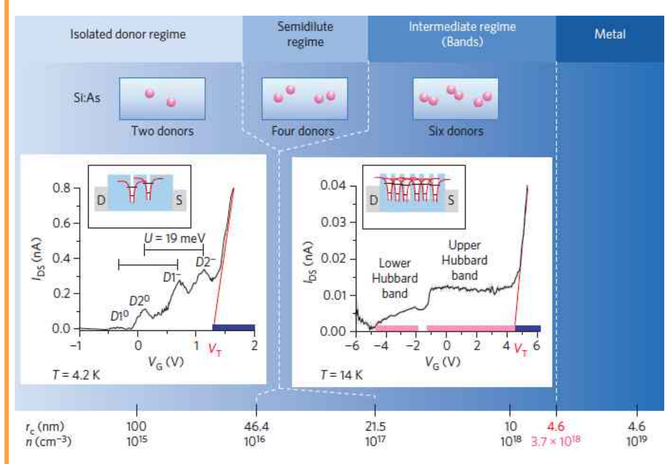
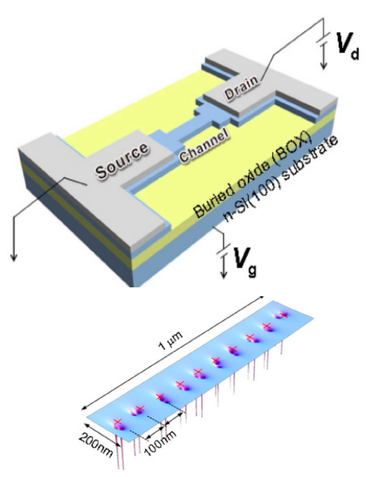
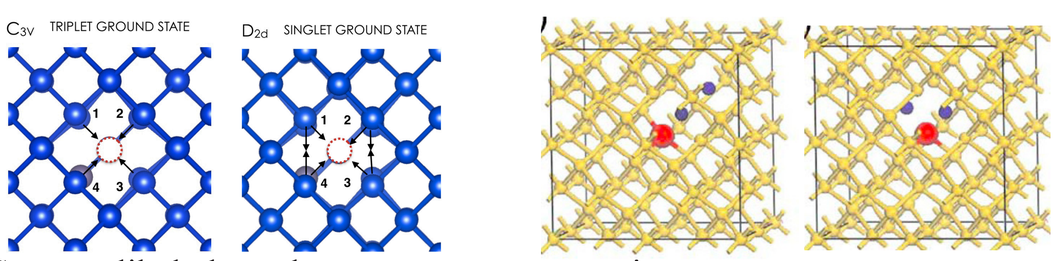
Single atom semiconductor devices based on conventional dopants (As, P) can only operate at cryogenic temperature because of electron ionization at room temperature. Differently, Ge implanted in Si and annealed at 500 °C behaves as a donor having deep levels in the bandgap [3,4]. Such system is a promising candidate to act as atomic center in silicon transistors up to room temperature. However, little is known about excited states and its potential role as coherent spin state center operating up to room temperature.
Our purpose is to apply the state of the art ab-initio density-functional based approaches to achieve a correct interpretation of the experimentally measured electronic and transport properties of Si with implanted Ge atoms. In particular we plan to apply hybrid functionals methods that are substantially less demanding than MBPT and allow to obtain quantitatively reliable results for quasiparticle levels together with good structural properties. This work is part of a Italy-Japan joined theoretical and experimental project presented to the NFFA.eu infrastructure.

DEVICE and EXPERIMENTAL DATA



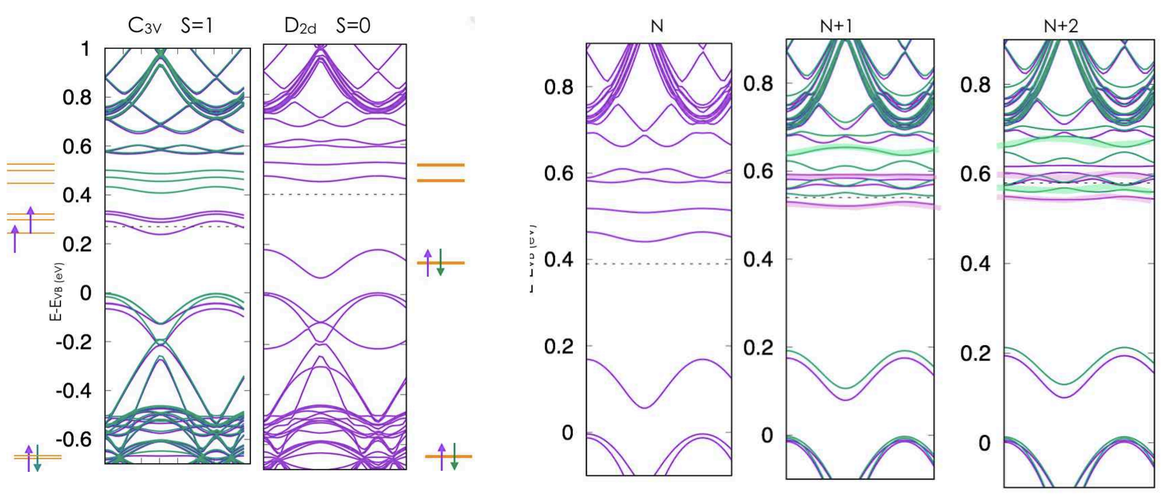


DEFECT GEOMETRY



Ge atom likely bound to one or more vacancies.
Geometrical relaxation at GGA level with SIESTA (pseudopotentials + localized atomic orbital basis set) large unit cell (64, 216, 360 atoms)

DFT ELECTRONIC PROPERTIES

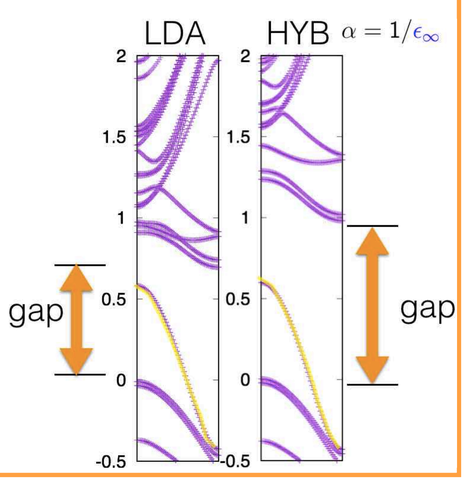


Ground state spin state depending on the local geometry
Defect states merging to CB in charged defect

$$\alpha\, E^{x}_{HF} + (\alpha-1)\, E^{x}_{DFT} + E^{c}_{DFT} \;\longrightarrow\; V_{Hybrid}$$

$$\alpha = 1/\epsilon_c$$

Preliminary calculations with hybrid potentials in the small cell (64 atoms) confirms the local geometry relaxation and improves the electronic properties description.



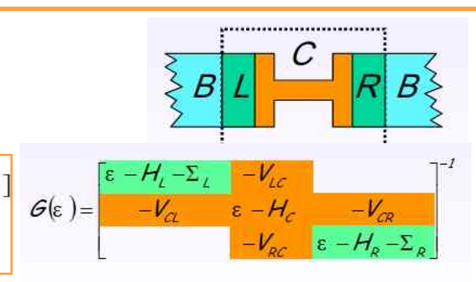
Recent results relative to electronic transport in nanostructures

- Electronic transport in balistic regime
- Non Equilibrium Green's function approach
- Transmission function T(E)= $\mathrm{Tr}[G^{\dagger}(\varepsilon)\Gamma_R(\varepsilon)G(\varepsilon)\Gamma_L$
- TRANSIESTA code (PRB 65,165401 (2002)

$$\Gamma_L(z) \equiv i[\Sigma_L(\varepsilon) - \Sigma_L(\varepsilon)^{\dagger}]/2$$

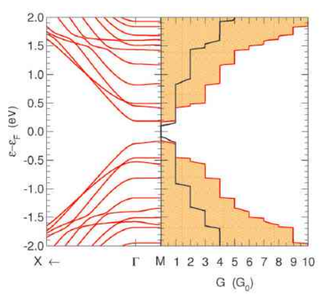
$$\Sigma_L(\varepsilon) \equiv [\mathbf{V}\mathbf{g}^{L}(\varepsilon)\mathbf{V}^{\dagger}]$$

$$I(V) = G_0 \int_{-\infty}^{\infty} d\varepsilon [n_F(\varepsilon-\mu_L) - n_F(\varepsilon-\mu_R)] \times \mathrm{Tr}[\Gamma_L(\varepsilon)\mathbf{G}^{\dagger}(\varepsilon)\Gamma_R(\varepsilon)\mathbf{G}(\varepsilon)],$$



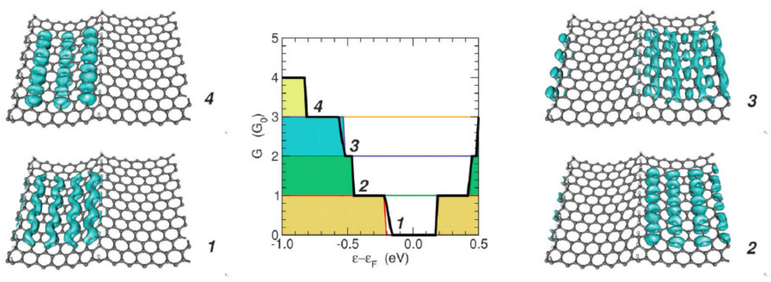
Hydrogen dimer lines and electron waveguides in graphene

S. Achilli, G. F. Tantardini and R. Martinazzo, Phys. Chem. Chem. Phys. 16, 17610 (2014)



- Hydrogen lines realize pseudo-nanoribbons.

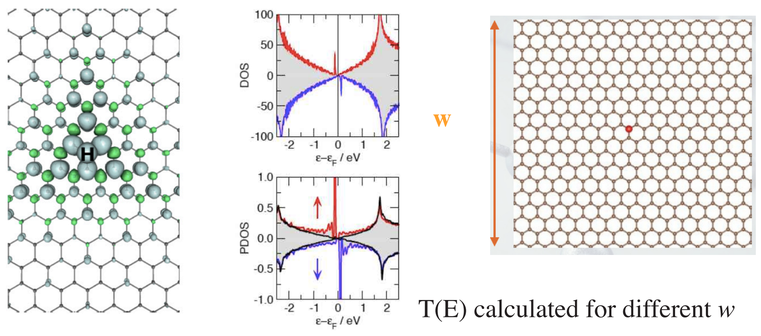
- Step-like T(E) related to localized states.



Transport eigenchannels show spatially localized electronic transport.

Firs principle semiclassical conductivity of neutral scatterers on graphene

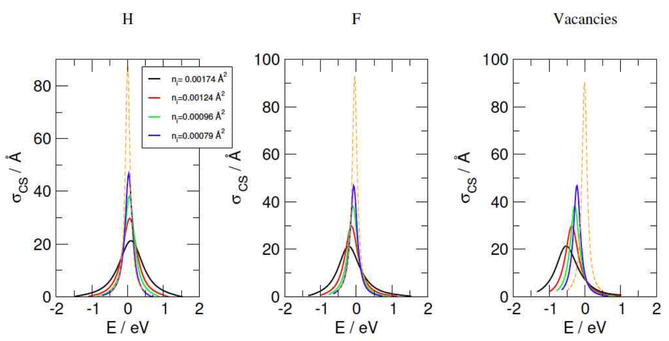
S. Achilli and R. Martinazzo,



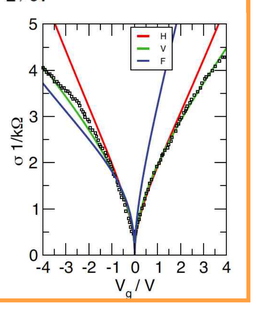
T(E) calculated for different w

$$\sigma_{DC} = \frac{4e_F^{\kappa}}{\pi h} w \frac{t}{r} = \frac{4e_F^{\kappa}}{\pi h} \frac{1}{n_i \sigma_{CS}} \qquad \sigma_{CS} = \frac{\pi}{2} w \frac{r}{t}$$

evaluated for different concentrations

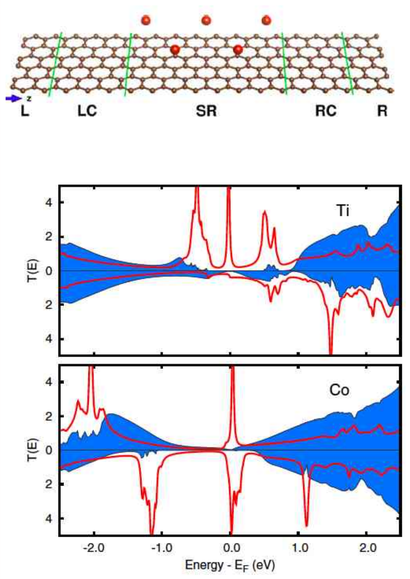


DC conductivity extracted in the limit of extremely low concentration.
Good agreement with experimental data (black dots)

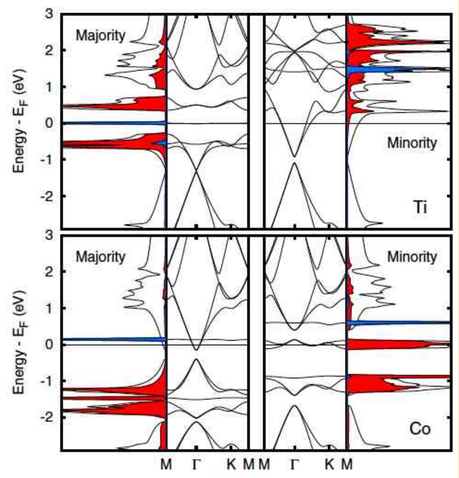


Spin filtering in graphene junctions with Ti and Co adsorbates

E. Del Castillo, S. Achilli, F. Cargnoni, D. Ceresoli, R. Soave, M. I. Trioni Chem. Phys. 478, 1 (2016)

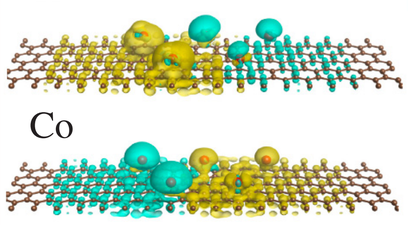


T(E) (blue) reflects spin dependent energy gap

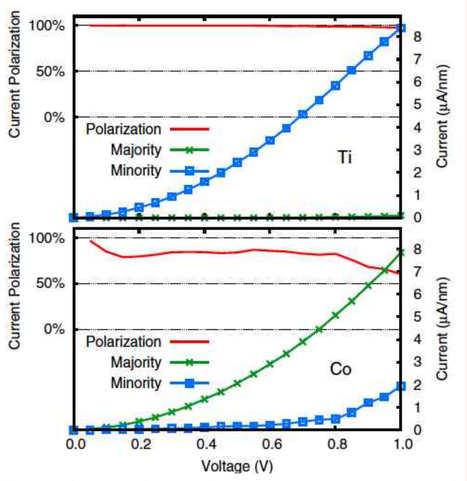


Band structure of Ti (Co)@graphene characterized by a majority (minority) spin energy gap

Ti
Co



Spin up (yellow) and down (green) electrons blocked by Ti and Co respectively



Spin dependent electronic current and current polarization