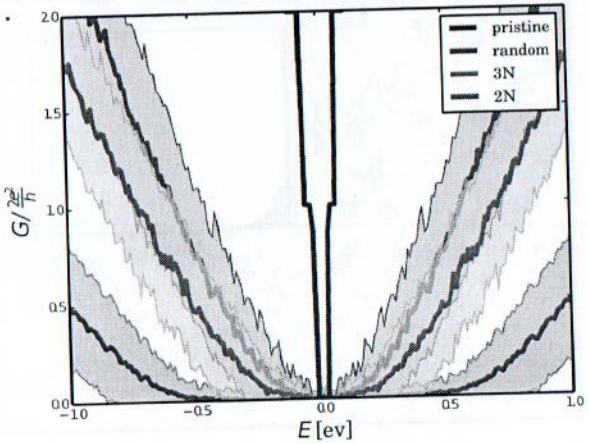
Quantum Transport

We cut nanoribbons from the simulation box and investigate quantum transport properties,
using the Landauer-Buttiker approach coupled to the Non Equilibrium Green Function (NEGF) formalism to investigate quantum transport .
We use the tight binding amiltonian (TB) of graphene

$$H = \sum_{<i,j>} t_{i,j} \left(a_i a_j^{\dagger} + h.c \right)$$

but set to zero all hoppings to and from carbon adatoms bonded to an hydorgen adatom.



We see that the conducatance for aggregated structures is much higher than the conductance obtained for a random distribution of H adatoms, as aggregation creates paths free of H adatoms trough the device, while being much lower than for pristine graphene.

Conclusions

H-H interactions

bound-counting model

up to 2N interactions ✗
up to 3N interactions ✓

Kinetic Monte Carlo

2N: long chain of H adatoms ✗
3N: sparse dendridic-like clusters ✓

Quantum Transport

aggregation increases conductance

Kinetic Simulations *and* Quantum Transport *in* Hydrogenated graphene

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Introduction

Graphene

Graphene is a novel 2D material made of carbon adatoms on an honeycomb lattice. It exibits an extrordinarly high conductibility and is an interesting candidate for post-silicon electronics. Yet to reach commercial applications a cheap technique to engineer a band gap is needed.

Hydrogenated graphene

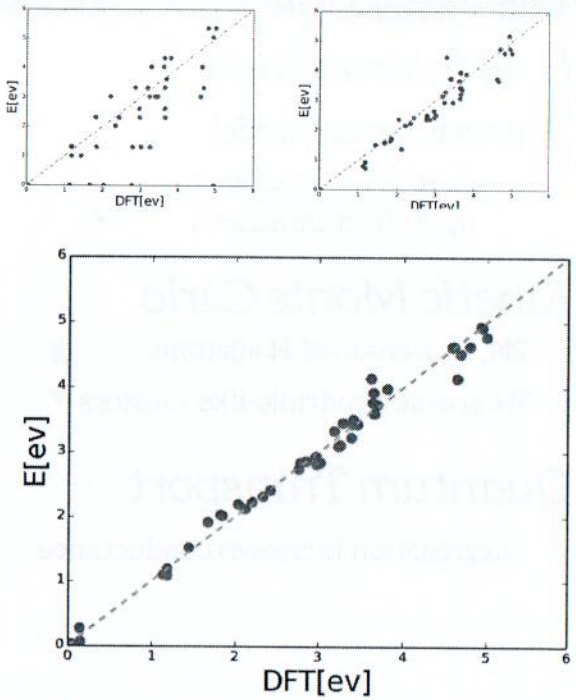
Hydrogen can adsorb onto carbon adatoms, changing the hybridization and thus changing the electronic structure of graphene, at the cost of an high adsorption energy barrier that makes difficult to reach an high H adrogen coverage.

As simulations of fully hydrogenated graphene (graphane, never experimentally achieved) show the precence of an high energy band gap, making this material interesting for applications. Experimentally and theoretically it has beeen shown that hydrogen adatoms interact strongly, leading to the formation of ordinated structures.

Aims

The goal of this thesis is to understand how hydrogen adatoms aggregate on the surface of graphene and how this aggregation affects quantum transport properties.

H-H interactions



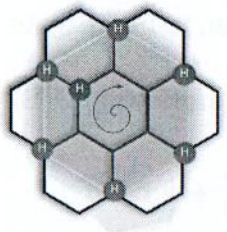
Neighboring H adatoms can form effective bonds with neighboring adatoms. We assume a short range interaction binding energy of form

$$E_b = \alpha_1 n_1 + \alpha_2 n_2$$
$$E_b = \beta_1 n_1 + \beta_2 n_2 + \beta_3 n_3$$
$$E_b = \gamma(n_1, n_2, n_3)$$

where n_1, n_2, n_3 are the number of first , second and third nearest neighbors and $\alpha_i, \beta_i, \gamma(n_1, n_2, n_3)$ are coefficients which we determined by comparison with DFT results, using the Simple Genetic Algorithm (SGA) to perform the fit. Whe show correlation plots in the figures, obtaining a good agreement only considering third-nearest neighbor (3N) interactions.

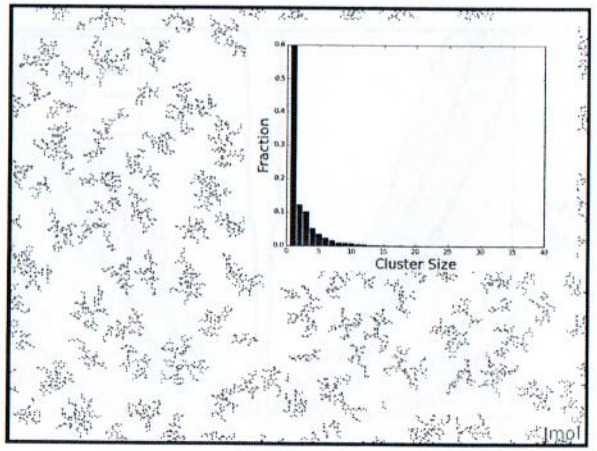
Kinetic Monte Carlo

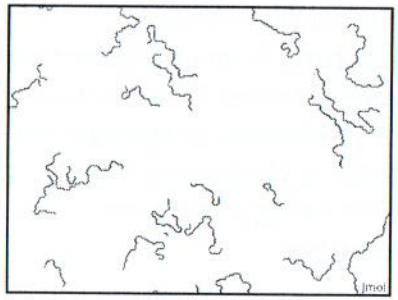
Using this model for H-H interactions we simulate the dynamics of hydrogen adatoms on graphene.
We implemented a Kinetic Lattice Monte Carlo algorithm to study the evolution of the system.



We were limited by the presence of kinetic traps, where on adatom (in red) loops for very long times on an exagon, trapped by other more stable hydrogens (orange).

We used Absorbing Markov Chain (AMC) theory to accellerate the algorithm. We find the configurations in the figure.





Neglecting 3N interactions we observe long chains, not seen by experiments.