

## Scientific Report “Short Visit Grant”

**Dr. Gianluca Stefanucci**

**Purpose of the visit:** We recently showed that the Kohn-Sham conductance overestimates the true conductance in the Coulomb blockade regime. This is due to the lack of dynamical exchange-correlation corrections. The purpose of the visit was to investigate the relation between these corrections and static DFT quantities of the molecular junction. In particular we intended to start from simple model systems and then extend the results to realistic systems.

**Description of the work carried out during the visit:** We obtained a simple formula to correct the Kohn-Sham conductance and benchmarked the formula against many-body calculations. We considered correlated junctions described by a tight-binding Hamiltonian, calculated the spectral function and then the many-body conductance. For the same system we calculated the corrected Kohn-Sham conductance and found very good agreement. We further studied the performance of our scheme in large systems like single-wall nanotubes quantum dots and compared the results with recent experimental data.

**Description of main results obtained:** The main result is the simple formula we derived to correct the Kohn-Sham conductance. This correction is especially important in molecules weakly coupled to leads where charging effects play an important role. The new formula is in good agreement with many-body calculations. Furthermore the comparison with experiments in single-wall nanotubes shows a neat improvement over the Kohn-Sham conductance, especially when the number of electrons in the junction is odd (open shell). Our results provide a full explanation of the Coulomb blockade effect without breaking the spin symmetry.

**Future collaboration with the host institution:** The progress we made during this week holds promise for important applications/extensions of the results obtained. We intend to implement the recently proposed exchange-correlation functionals with a derivative discontinuity and improve the calculation of the dynamical XC correction in closed shell molecular junctions. It is therefore our intention to continue the collaboration possibly with other short visits.

**Projected publications:** We are going to submit a first paper this month. A long and more detailed version of the paper will instead appear this year.