International Conference on Quantum Energy 2025 hosted by Dipartimento di Fisica e Astronomia Galileo Galilei an event by ICQE

Contribution ID: **77** Type: **Invited**

Spin-polarized electron transport through nanojunctions

Thursday 5 June 2025 10:40 (30 minutes)

The conductance properties of nanojunctions connected to macroscopic electrodes can be explored through quantum transport calculations that employ non-equilibrium Green's functions (NEGF) alongside density functional theory (DFT). When these systems exhibit electron spin polarization, the theoretical analysis often incorporates spin-polarized or unrestricted DFT. In this contribution, we present several examples of nanostructures where this approach has proven effective. First, we examine spin-polarized currents in zigzag graphene nanoribbons (zGNRs) subjected to
electric fields and finite bias voltages.[1] Next, we explore electron transport through molecules with unpaired electrons, in particular oxidized molecules that demonstrate highly conductive low-energy states, classified as one-dimensional topological insulators.[2] It is well-known that DFT can encounter difficulties with open-shell structures due to their multiconfigurational nature. We illustrate how a selection of polycyclic aromatic hydrocarbons—such as those previously studied in recent scanning probe experiments [3]—can have their ground state accurately determined using a multi- configurational short-range DFT approach.[4] Our findings underscore both the effectiveness and the limitations of integrating DFT with NEGF calculations.

Theme

Primary author: Prof. LEITHERER-STENGER, Susanne (University of Copenhagen)

Presenter: Prof. LEITHERER-STENGER, Susanne (University of Copenhagen)

Track Classification: Theme 3. Theoretical and experimental methods for quantum effects in energy processes