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EINLADUNG zum IFP-SEMINAR

Electrode effects on the observability of destructive quantum interference in single-molecule junctions

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Host: Christoph Eisenmenger-Sittner

Termin: Mittwoch, 18. Jänner 2023, 16:00 Uhr

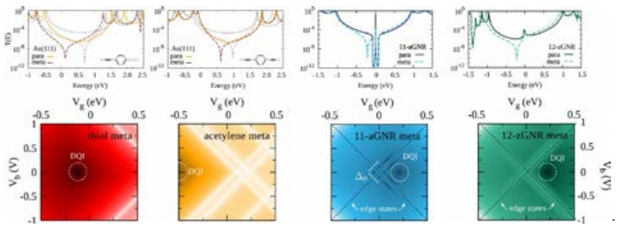
Ort: Institut für Festkörperphysik, TU Wien

Wiedner Hauptstraße 8-10, 1040 Wien

Seminarraum DC rot 07 (roter Bereich, 7. OG)

Abstract:

Destructive quantum interference (QI) has been a source of interest as a new paradigm for molecular electronics as the electronic conductance is widely dependent on the occurrence or absence of destructive QI effects. In order to interpret experimentally observed transmission features, it is necessary to understand the role played by all components of the junction, including the molecular core, the linkers, and the electrodes. First principle calculations allow assessing the structure-function relation for quantum transport through pyrene molecular junctions with distinct QI properties, and to capture a complexity that is beyond simple Hückel model calculations. A thorough analysis allows to disentangle the transmission features arising from the molecule and the electrodes and determine the observability of destructive QI. We also suggest that QI can be relevant for chemical sensing. The adsorption of small gaseous molecules (NO_2, H_2O, and NH_3) on pyrene is systematically investigated varying the adsorption site and adsorbate orientation in order to understand the selectivity properties of graphene-like junctions. Our study can potentially be useful for developing graphene-based sensors exploiting QI effects.



References:

-Sengul, O., Valli, A., & Stadler, R. (2021). Electrode effects on the observability of destructive quantum interference in single-molecule junctions. Nanoscale, 13(40), 17011-17021.

-Sengul, O., Völkle, J., Valli, A., & Stadler, R. (2022). Enhancing the sensitivity and selectivity of pyrene-based sensors for detection of small gaseous molecules via destructive quantum interference. Physical Review B, 105(16), 165428