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TÉMA

Mechanically-tunable quantum interference in ferrocene-based molecular junctions

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Ferrocene is a well-known organometallic 'sandwich' compound made of one iron atom between two cyclopentadiene (Cp) rings. Inspired by recent experimental scanning tunneling microscope break junction measurements, I will present the results of an extensive computational study of transport properties of ferrocene and ferrocene-based molecular junctions. Using density functional theory and non-equilibrium Green's function formalism, I show that the transmission function presents a combination of sharp Fano-type resonances as well as anti-resonances close to Fermi energy. The anti-resonances are pronounced and wide, and can be used to explain the experimental results.

Moreover, rotating the rings against each other orbital hybridization (and thus quantum interference) can be controlled mechanically with conductance changing by orders of magnitude.

I will also show an effective three-level tight-binding model, which rationalizes our numerical findings, and emphasizes the critical role of the symmetries of the molecular orbitals in the quantum interference.

odborný garant: *Hector Vazquez, Ph.D.*.