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Aula del edificio I+D+i

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Unraveling the Interplay between Quantum Transport and Geometrical Conformations in Molecular Junctions

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In molecular electronics transport experiments performed using the break-junction (BJ) approach, identifying the orientation of the molecule between the nanoelectrodes is a challenging task. To uncover the relationship between the orientation of the molecule and its conductance, we have combined experimental results obtained via the BJ technique with atomistic simulations and ab initio calculations. The results we will present cover both helicene-type [1] molecules and solvents such as monocyclic hydrocarbons [2,3].

Our experimental results reveal how electronic transport occurs when a molecule is captured and stretched between two electrodes. Additionally, results from classical molecular dynamics (CMD) simulations have shown the most common orientations of organic molecules under these conditions. Furthermore, for all simulated cases, we have calculated electronic transport using Density Functional Theory (DFT) calculations.

Thanks to the good agreement between experimental and theoretical results, we can conclude that it is possible to uncover the relationship between molecular orientation and electronic transport for both simple solvents like benzene, toluene, and cyclohexane, as well as for helicoidal molecules such as dithia[n]helicenes.

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