Spin-dependent conductance switching in organic molecular junctions

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We use density-functional theory to calculate the electronic transport through single molecules attached to capped (5,5) carbon nanotubes (CNTs) as leads.

We observed a strong variation in the electrical conductance with respect to the spin-state of the junction. The singlet state exhibits high conductance whereas the triplet low. The deformation of the CNTs' cap structure, upon covalent adsorption of the phenyl rings, triggers the spin dependence in the organic junctions. Two different π-conjugated phenylene-vinylene-containing molecules were tested, yielding similar behavior.

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