Pathways in molecular conductance and spin coupling

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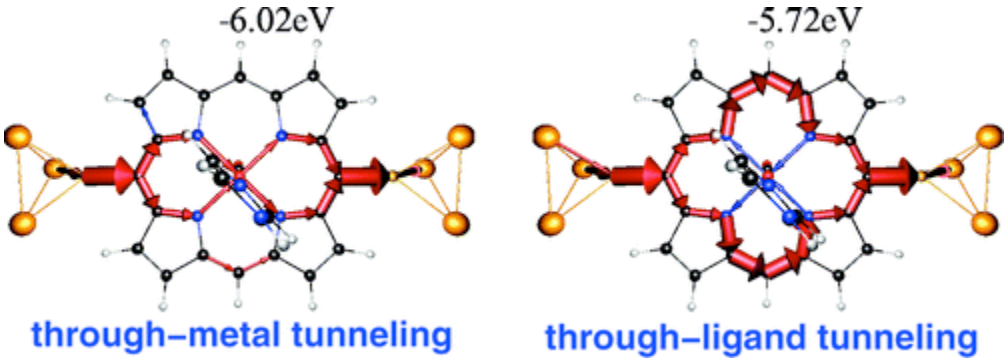
For understanding spin-polarized electron transport through molecular bridges and (exchange) spin coupling between local spin centers within in a molecule, it is interesting to know which parts of the molecule are responsible for mediating transport or spin interactions.

In the case of spin coupling, ferro- and antiferromagnetic pathways may add up or partially cancel, which is hidden if only the total spin coupling is considered. A new approach to decomposing spin coupling based on Green's functions[1] allows not only identifying which molecular parts are responsible for spin coupling in isolated molecules, but may also allow for distinguishing, e.g., between intramolecular and through-surface contributions[2].

In electron transport through molecular junctions, local decomposition of electron transmission will be used to highlight the importance of spin-polarized parts of the molecule for transport[3-7], and compared with the effect of introducing spin polarization in bridging ligands on spin coupling[8].



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