

# Spin-philicity and spin-donicity as auxiliary concepts to quantify spin-catalysis phenomena

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For molecular systems susceptible to undergo a change of their spin state as a result of a chemical reaction with a given reactant, the spin-polarized density functional theory is used to define the concepts of "spin-philicity" ( $\chi^S +$ ) and "spin-donicity" ( $\chi^S -$ ) as global reactivity indexes. They are defined as the maximum energy change when a molecular system acquires or donates a spin number  $\Delta N_S$  to increase ( $\chi^S +$ ) or decrease ( $\chi^S -$ ) its spin multiplicity. The spin transformation of chemically reactive species induced by the interaction of these molecules with external spin carriers—a phenomenon known as spin catalysis—is discussed on the basis of an absolute scale for  $\chi^S +$  and  $\chi^S -$ . As an illustration of the method, a selection of paramagnetic and diamagnetic molecules, commonly used as spin catalyst, is classified within this scale and the hierarchy obtained is compared with the available experimental information.