On the principle of spin potential equalization

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In analogy with Sanderson's electronegativity equalization principle, it is possible to postulate a principle of spin potential equalization in the E[N?, N?] representation of the spin polarized density functional theory, where N? and N? refer to the number of electrons with spins ? and ?, respectively. The principle provides simple expressions to evaluate the energy changes AE between two interacting molecules, A and B, together with the electron transfer, ?N? and ?N?. The model is illustrated for a series of addition reactions of electrophilic, nucleophilic, and ambiphilic carbenes to alkenes in their singlet and triplet multiplicities. The results are in a consistent qualitative agreement with the experimental reactivity established for these systems.