

## Chemical reactivity in the $\{N, NS, v(r)\}$ space

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A reactivity picture developed within the spin-polarized density functional theory defined in the  $E\{N, NS, v(r)\}$  space is discussed. The reactivity model including changes in the total number of electrons  $N$ , the spin number (unpaired electron number)  $NS$ , and the external potential  $v(r)$  is tested against two chemical processes involving radical species. They are the hydrogenation reaction of the succinimidyl radical and the Bergman cyclization. Although the former reaction appears to be mostly driven by the spin potential, a quantity measuring the variations in electronic energy with respect to the spin multiplicity changes; the latter presents highly electrocyclic character without significant spin-polarization effects.