Estimation of effective exchange integral value of polyradical systems based on the band calculation

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We have utilized to elucidate effective exchange integral (J_{ab}) vales between local spins, which are defined by the Heisenberg model. In recent years, mesoscopic systems have attracted much attention in a material science. In polyradical systems, the J_{ab} values are presented as follow

$$J_{\mathrm{ab}} = \frac{E^{\mathrm{LS}} - E^{\mathrm{HS}}}{\left\langle \hat{S}^2 \right\rangle^{\mathrm{HS}} - \left\langle \hat{S}^2 \right\rangle^{\mathrm{LS}} + c}$$

where E^{X} , $\left\langle \hat{S}^2 \right\rangle^{\mathrm{X}}$ and c are total energy, total spin angular momentum of spin state X (X= low-spin (LS) and high-spin (HS) states) and a correction constant, respectively. A periodic system is utilized to elucidate the J_{ab} value to use a periodic boundary condition. A purpose of this study is to estimate the J_{ab} value with band theory to periodic one-dimensional polyhydrogen radicals and a polymethyl radials.

A result of polyhydrogen is shown Fig 1. In AP and Ising, we make an estimate of the J_{ab} value of a mesoscopic hydrogen cluster composed of 100 hydrogen atoms H_{100}. The J_{ab} value of band theory is defined a half of S-T gap. Results of Ising and band theory are same J_{ab} values.

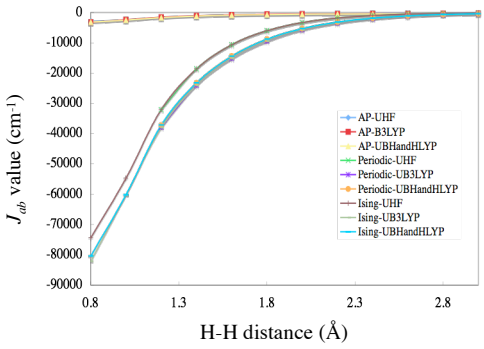

Fig 1. The J_{ab} value of polyhydrogen radicals