Supplementary Material (ESI) for PCCP

Electronic Supplementary Information (ESI) for

Pathway Analysis of Super-exchange Electronic Couplings in Electron Transfer Reactions by Using a Multiconfiguration Self-consistent Field Method

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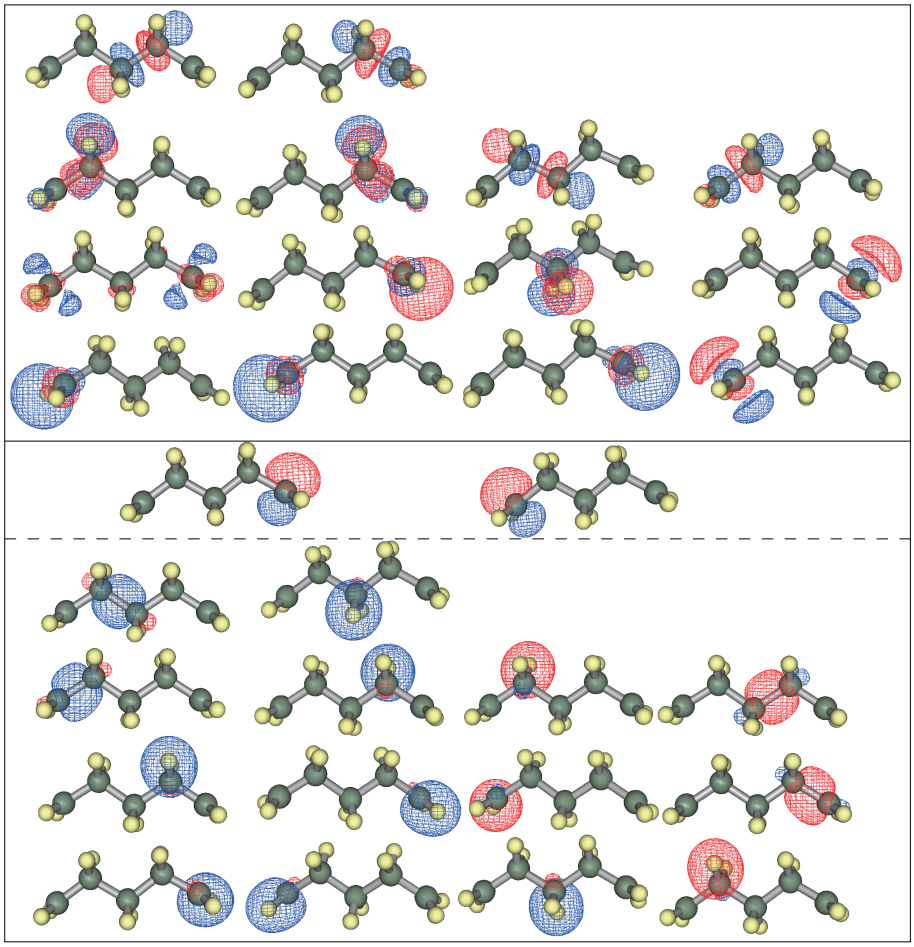

Fig. S1 Same as Fig. 3 but for pentane-1,5-diyl anion.

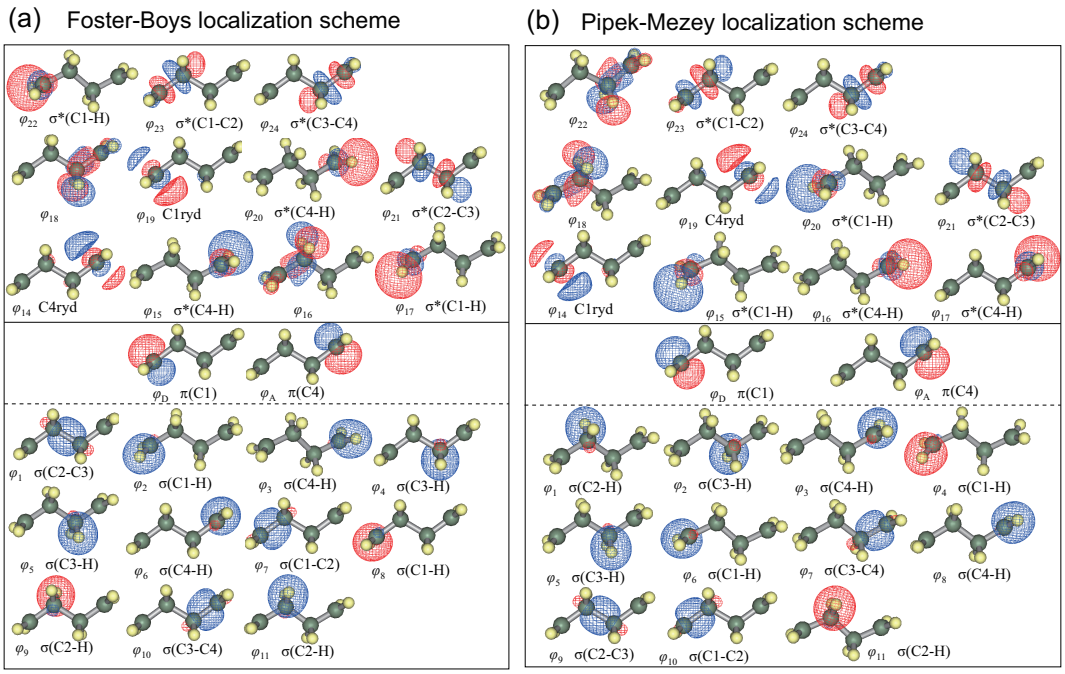

Fig. S2 Same as Fig. 3 but with (a) the Foster-Boys localization scheme and (b) the Pipek-Mezey localization scheme.

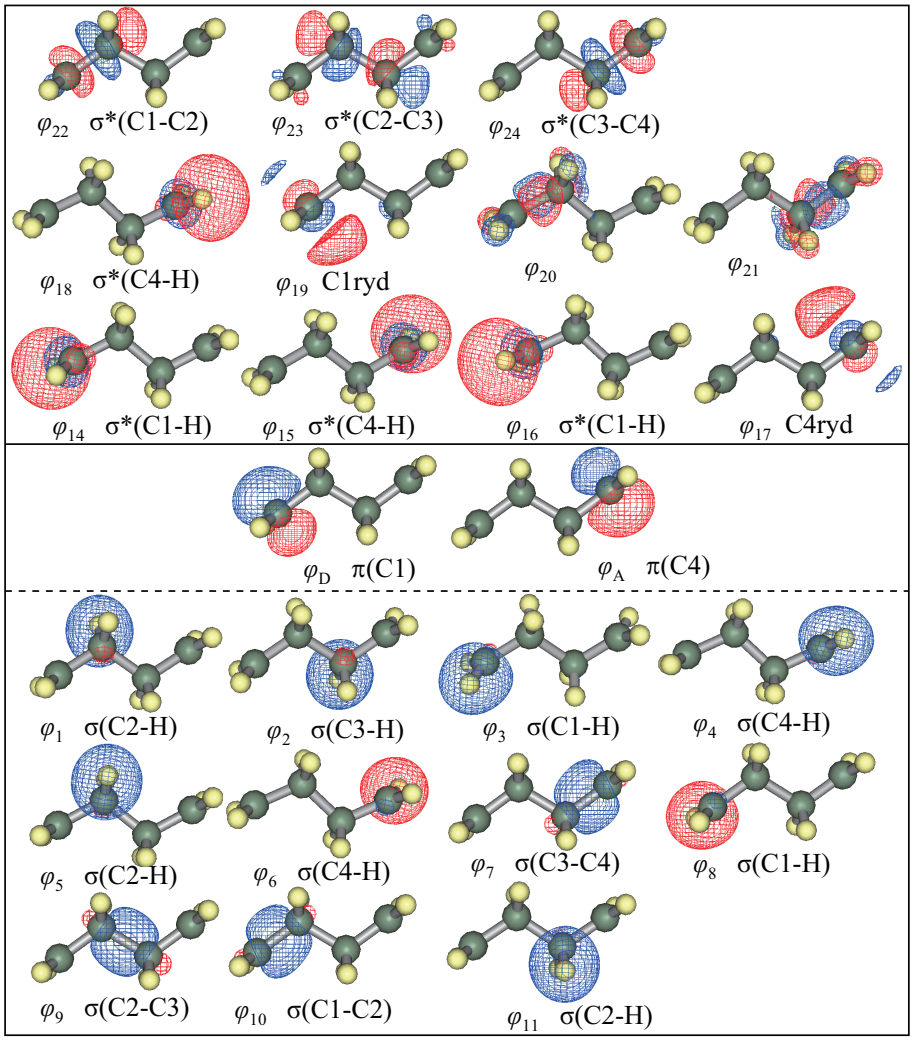

Fig. S3 Same as Fig. 3 but with the 6-31G(d) basis set.

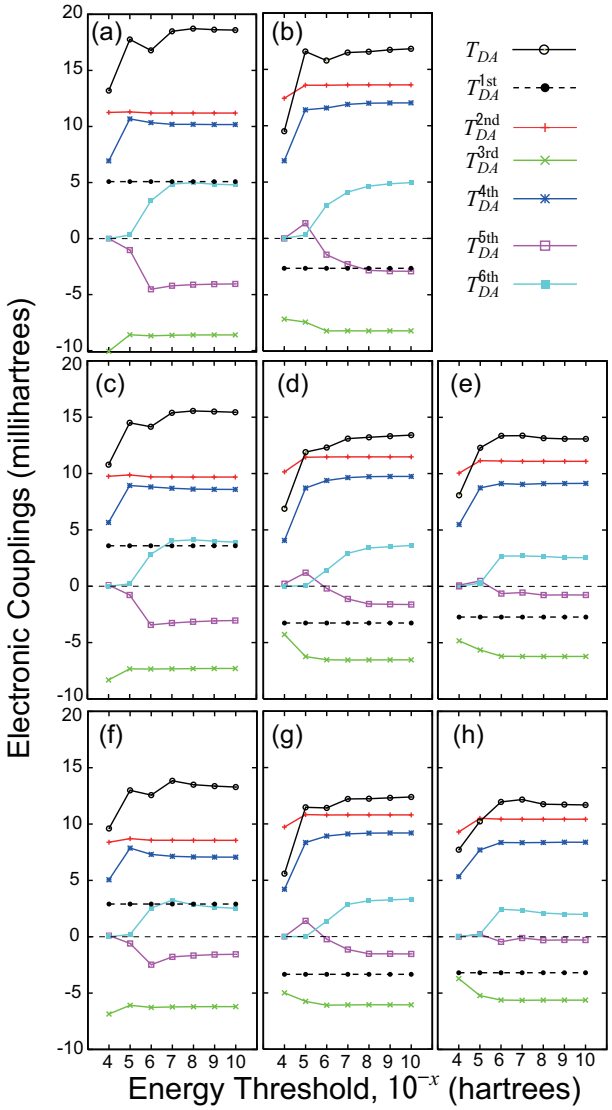

Fig. S4 Same as Fig. 4 but with the basis set / localization scheme of (a) 3-21G / Pipek-Mezey, (b) 3-21G / Foster-Boys, (c) 6-31G(d) / Pipek-Mezey, (d) 6-31G(d) / Foster-Boys, (e) 6-31G(d) / Edmiston-Ruedenberg, (f) cc-pVDZ / Pipek-Mezey, (g) cc-pVDZ / Foster-Boys, and (h) cc-pVDZ / Edmiston-Ruedenberg.

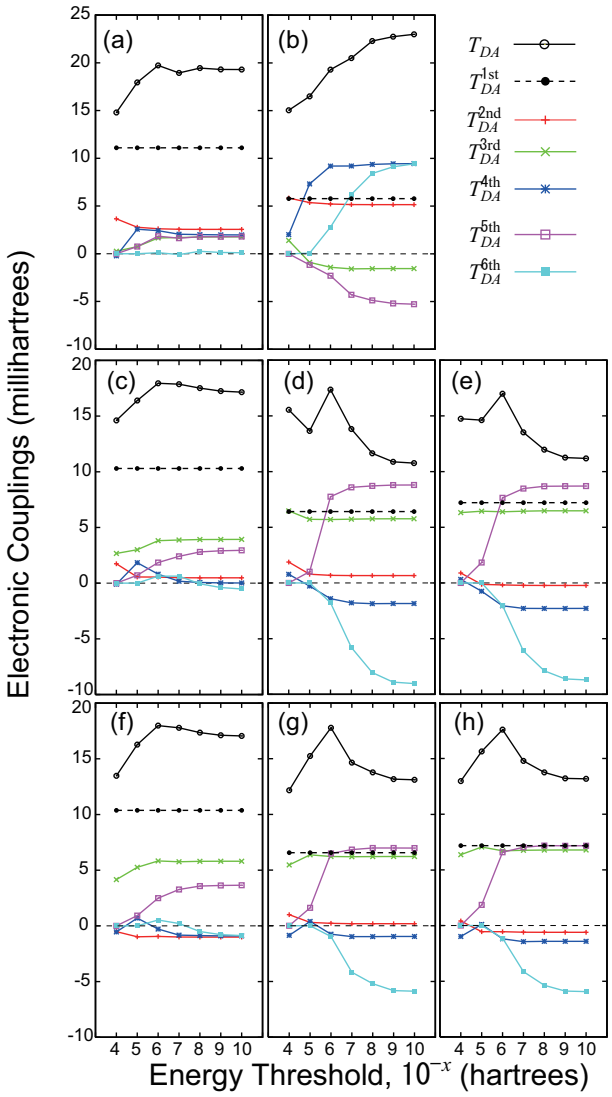

Fig. S5 Same as Fig. S4 but for anion coupling of pentane-1,5-diyl.

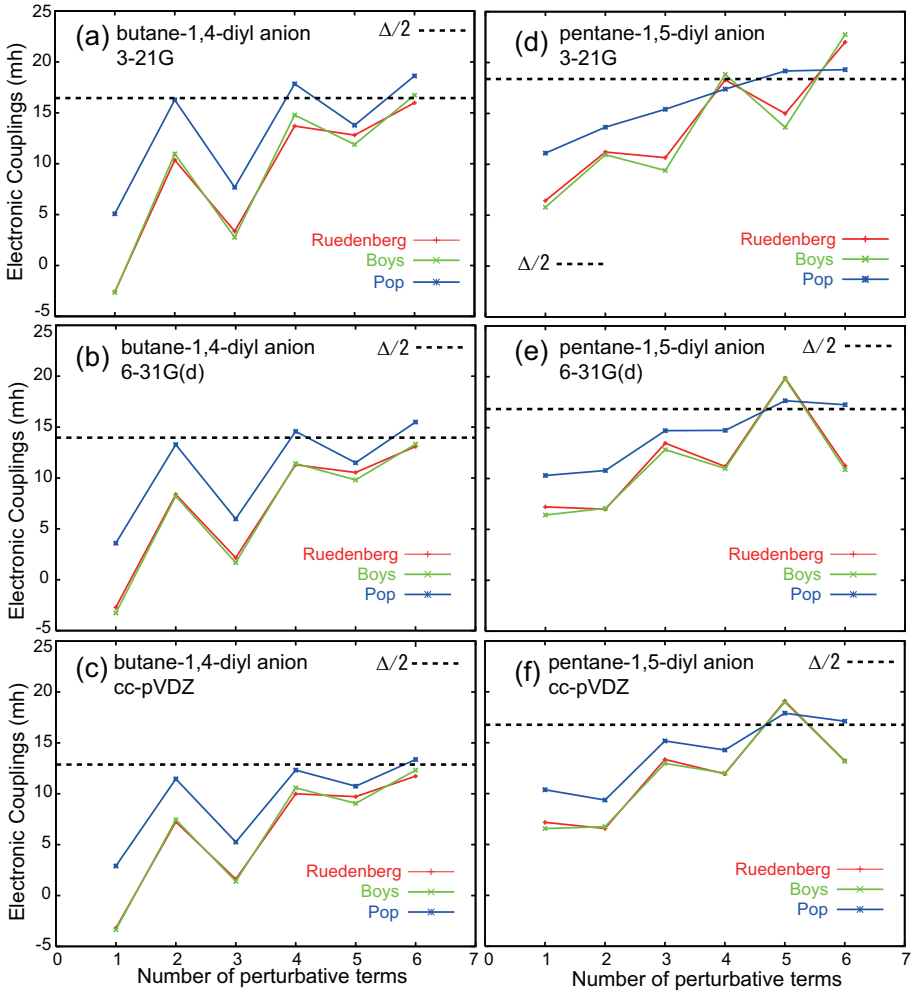

Fig. S6 Dependence of T_{DA} from eqn 15 on the number of perturbative terms with the energy threshold of 10^{-9} hartree.

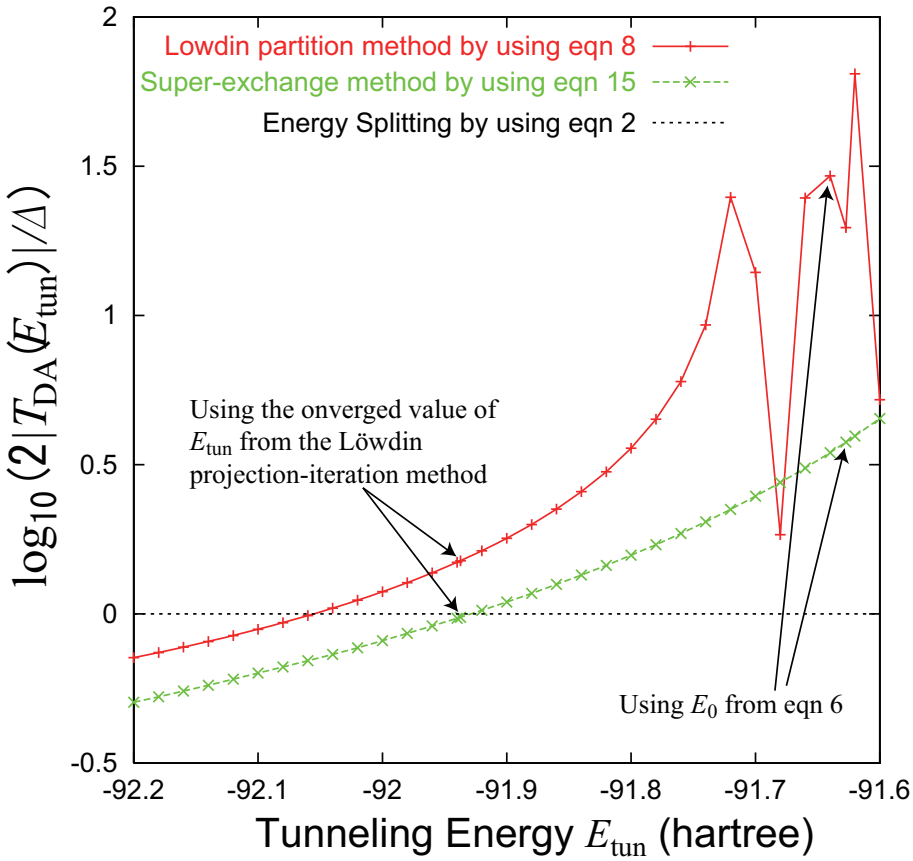

Fig. S7 Dependence of $H_{DA}^{\rm eff}$ from eqn 8 and T_{DA} from eqn 15 on the tunneling energy $E_{\rm tun}$ for butane-1,4-diyl anion. The Ruedenberg localization scheme with the 3-21G basis set was used. The energy threshold of 10^{-8} hartree was employed for the higher-order super-exchange calculation (eqn 15).

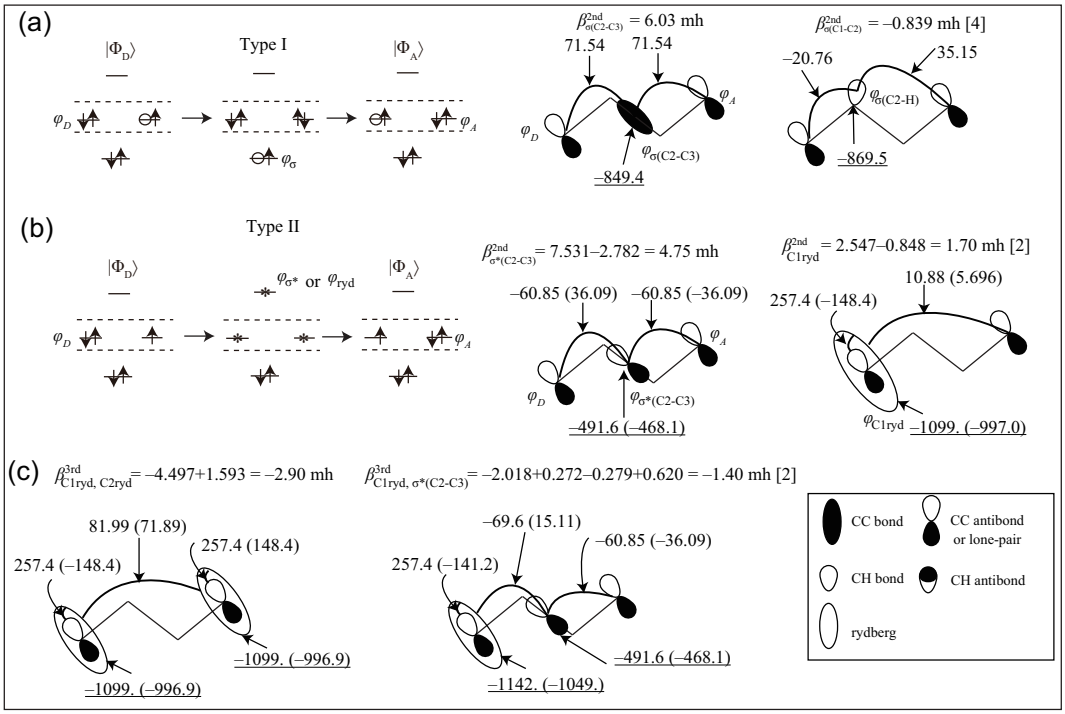

Fig. S8 Same as Fig. 6 but with the Pipek-Mezey localization scheme.

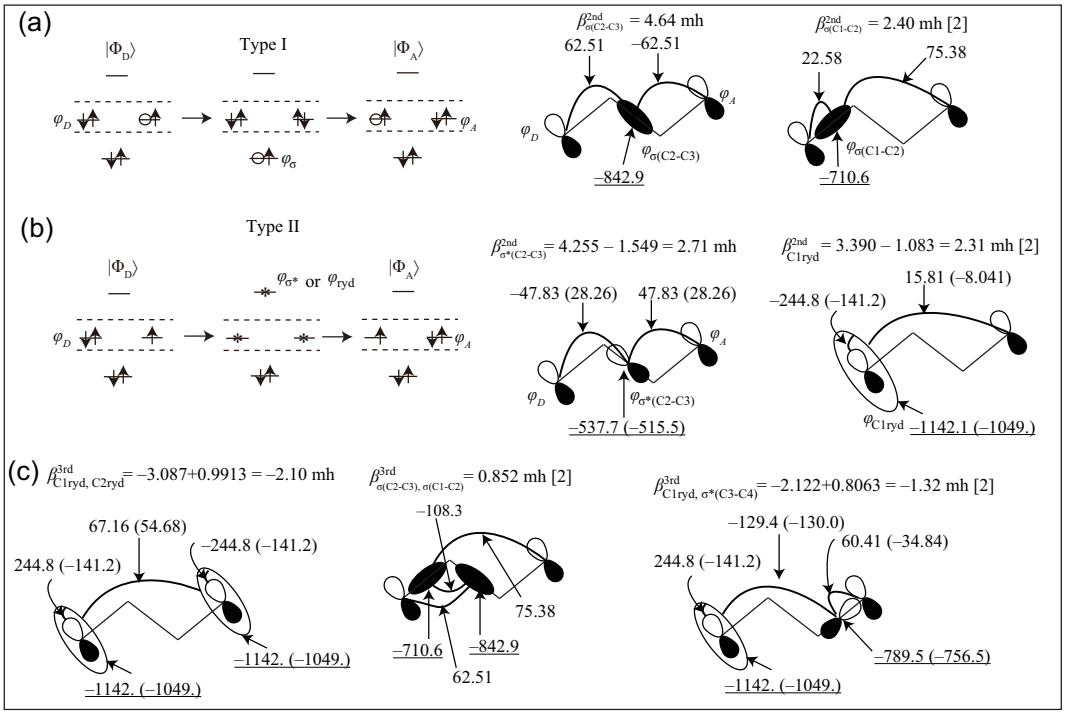

Fig. S9 Same as Fig. 6 but with the Foster-Boys localization scheme.

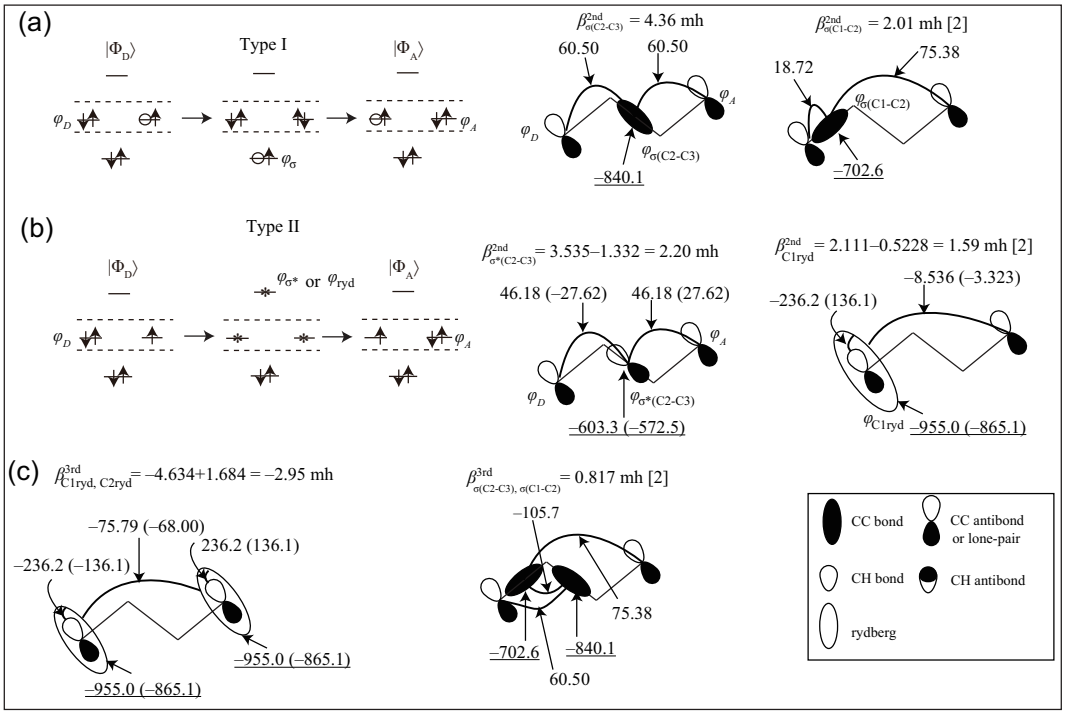

Fig. S10 Same as Fig. 6 but with the 6-31G(d) basis set.

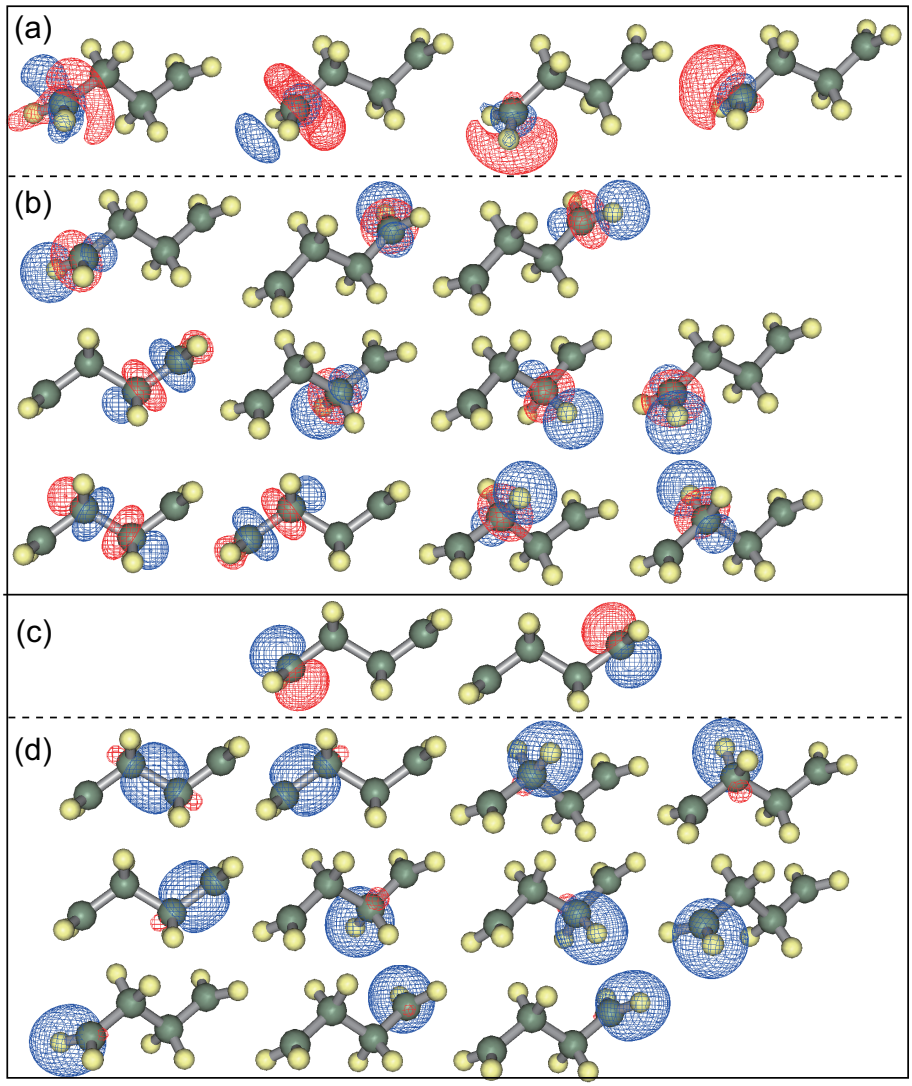

Fig. S11 The NBOs with the 3-21G basis set for neutral triplet state of butane-1,4-diyl. (a) NBOs correspond to the extra-valence-shell orbitals at C1. The orbital groups (b) (c), and (d) correspond to (a), (b), and (c) in Figure 3.