Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Orbital-based insights into parallel-displaced and twisted conformations in π-π interactions

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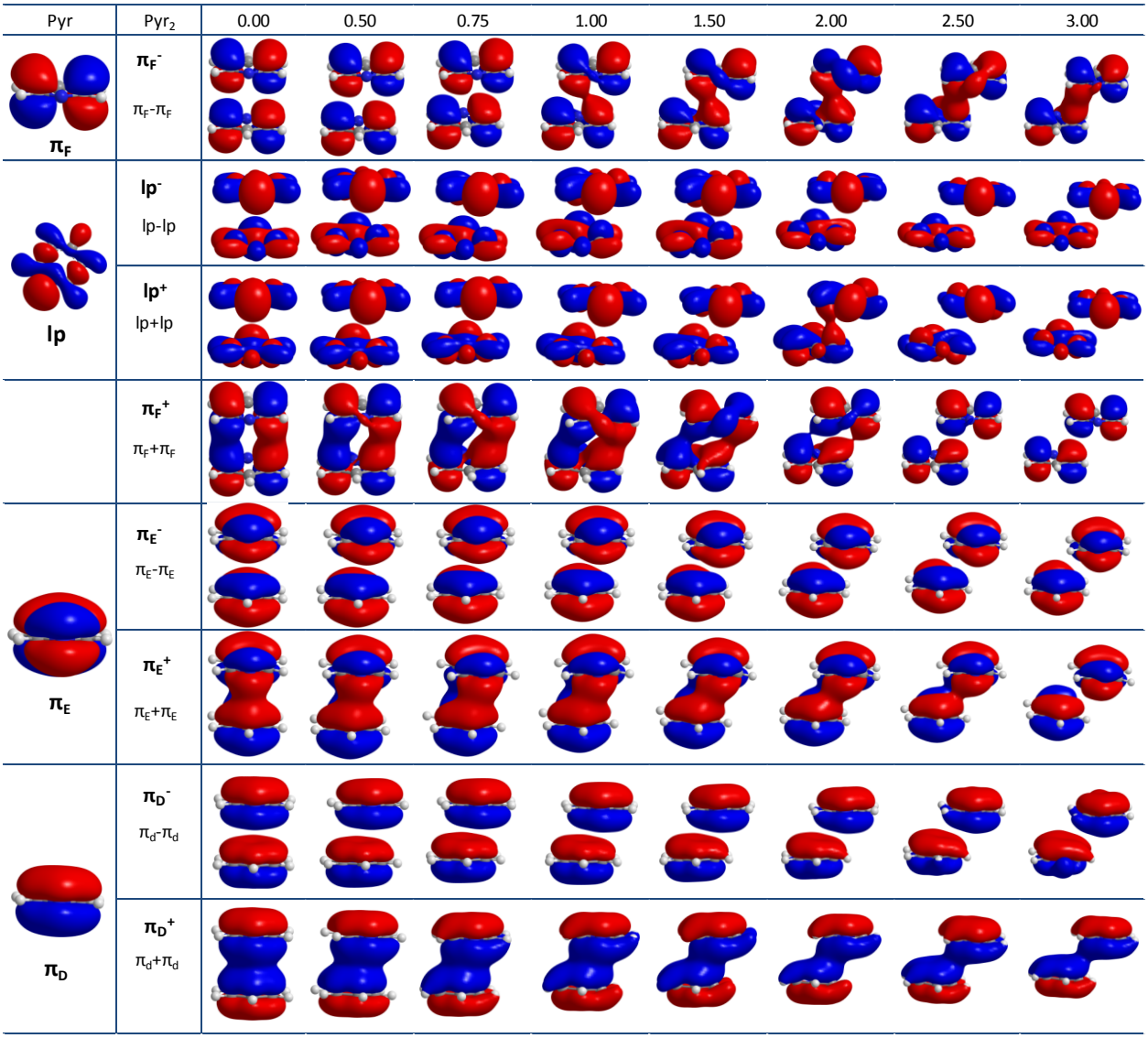

Figure S1. The orbital representations of the top four π molecular orbitals of Pyr_2 as a function of R_{slip}.

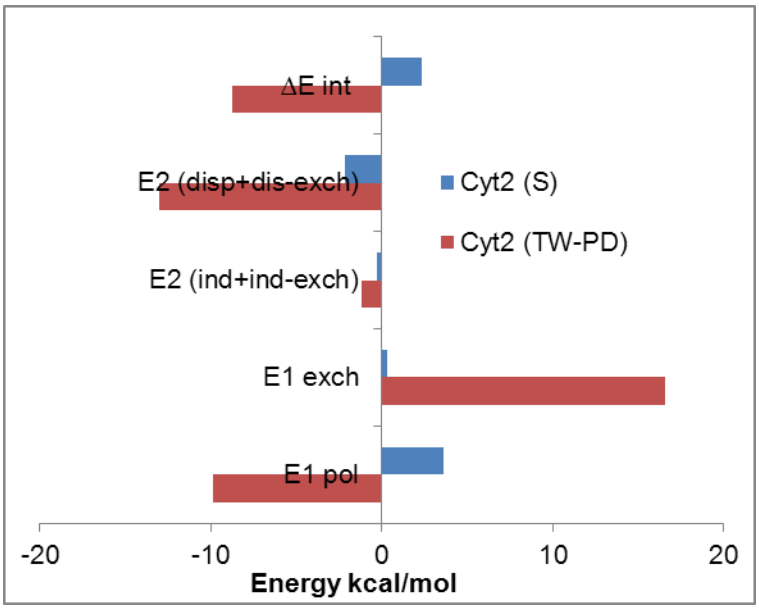

Figure S2. DF-DFT-SAPT energy contributions for both Cyt_2 (S) and Cyt_2 (TW-PD**).**

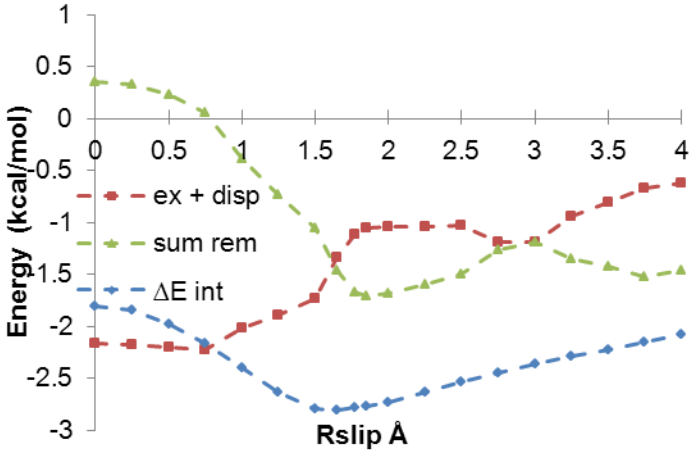

Figure S3. Plot of the DF-DFT-SAPT E_{int}, the sum of the $E_{exch}^{(1)}$ and $E_{disp}^{(2)}$ contributions, and the sum of the remaining $E_{pol}^{(1)}$, $E_{ind}^{(2)}$, $E_{ind\text{-}disp}^{(2)}$, $E_{exch\text{-}disp}^{(2)}$and δ(HF) terms for Bz_2 plotted as a function of R_{slip}.

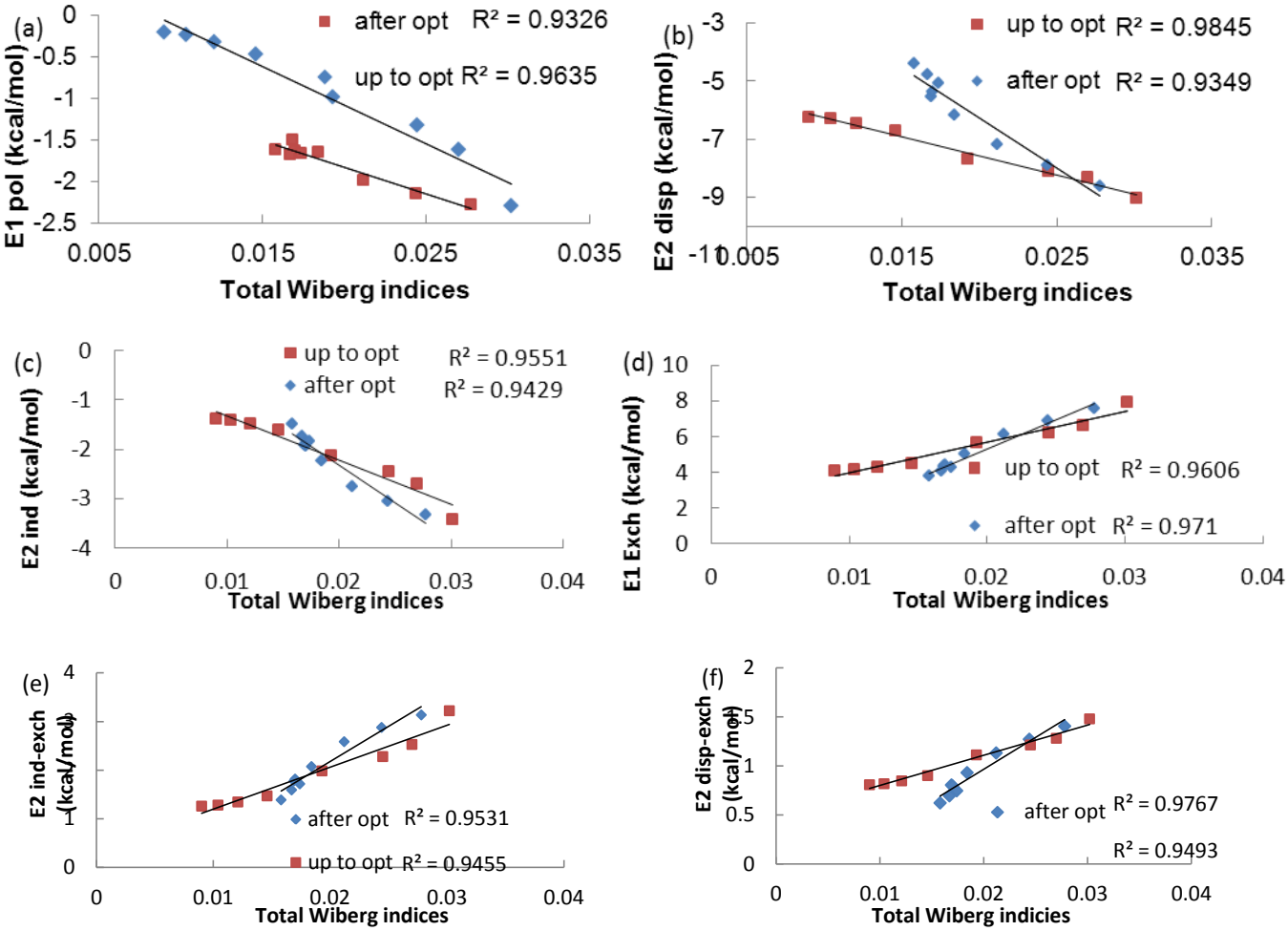

Figure S4. DF-DFT-SAPT energy contributions for Bz_2 plotted as a function of the total intermolecular Wiberg bond indices which displays a change in slope before and after the minimum reflecting a change in the type of momomer MOs involved in inter-ring bonding. **(**a) Plot of $E_{pol}^{(1)}$ as a function of the total WBI. **(**b) Plot of $E_{disp}^{(2)}$ plotted as function of total WBI. (c) Plot of $E_{ind}^{(2)}$ as a function of the total WBI. (d) Plot of $E_{exch}^{(1)}$ as a function of the total WBI. (e) Plot of $E_{ind\text{-}exch}^{(2)}$ as a function of the total WBI. **f**, Plot of $E_{disp\text{-}exch}^{(2)}$ as a function of the total WBI.

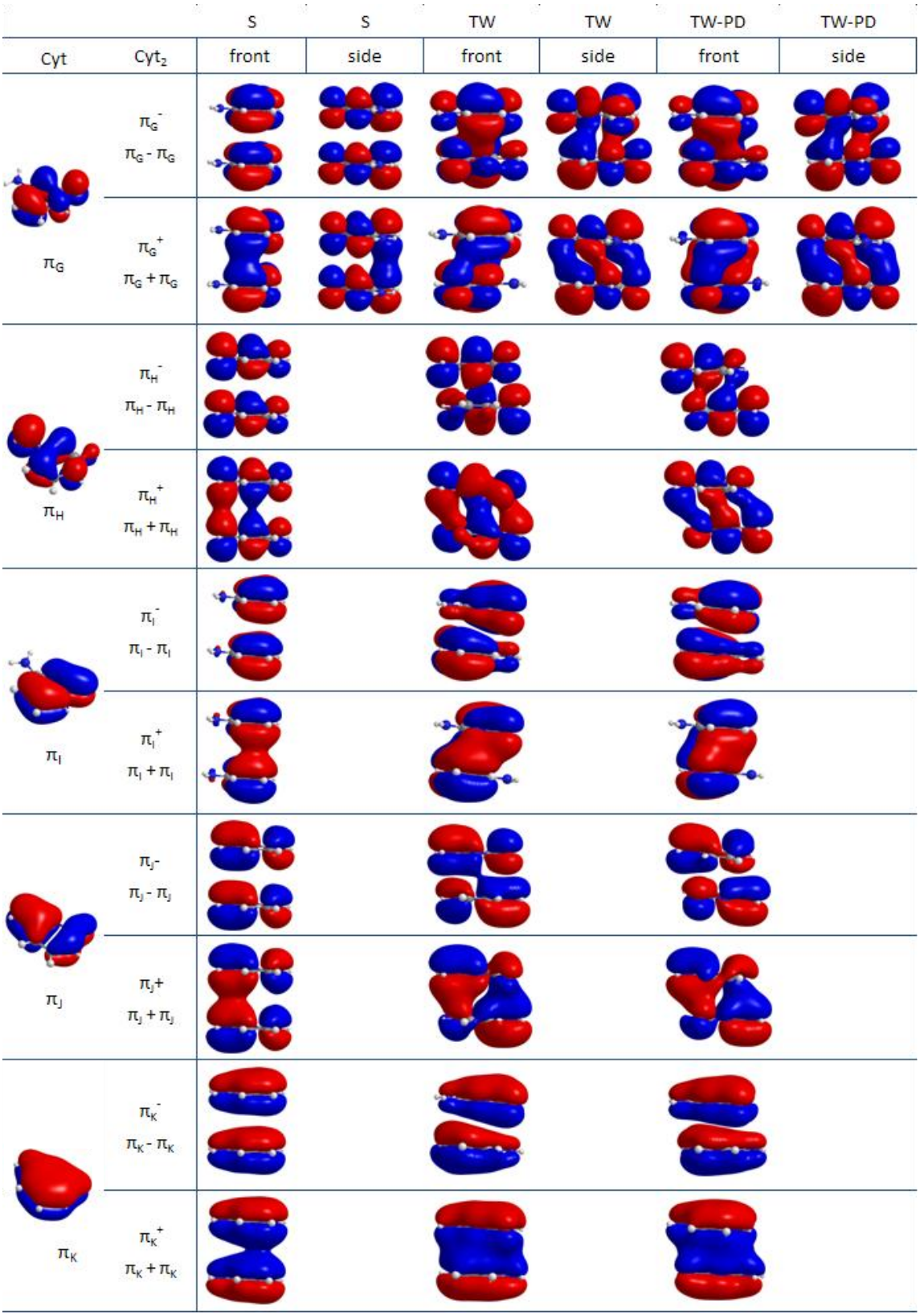

Figure S5. The orbital representations of the 10 π orbitals for Cyt_2.