

Supporting Information for

“Singlet Fission in Pancake-Bonded Systems”

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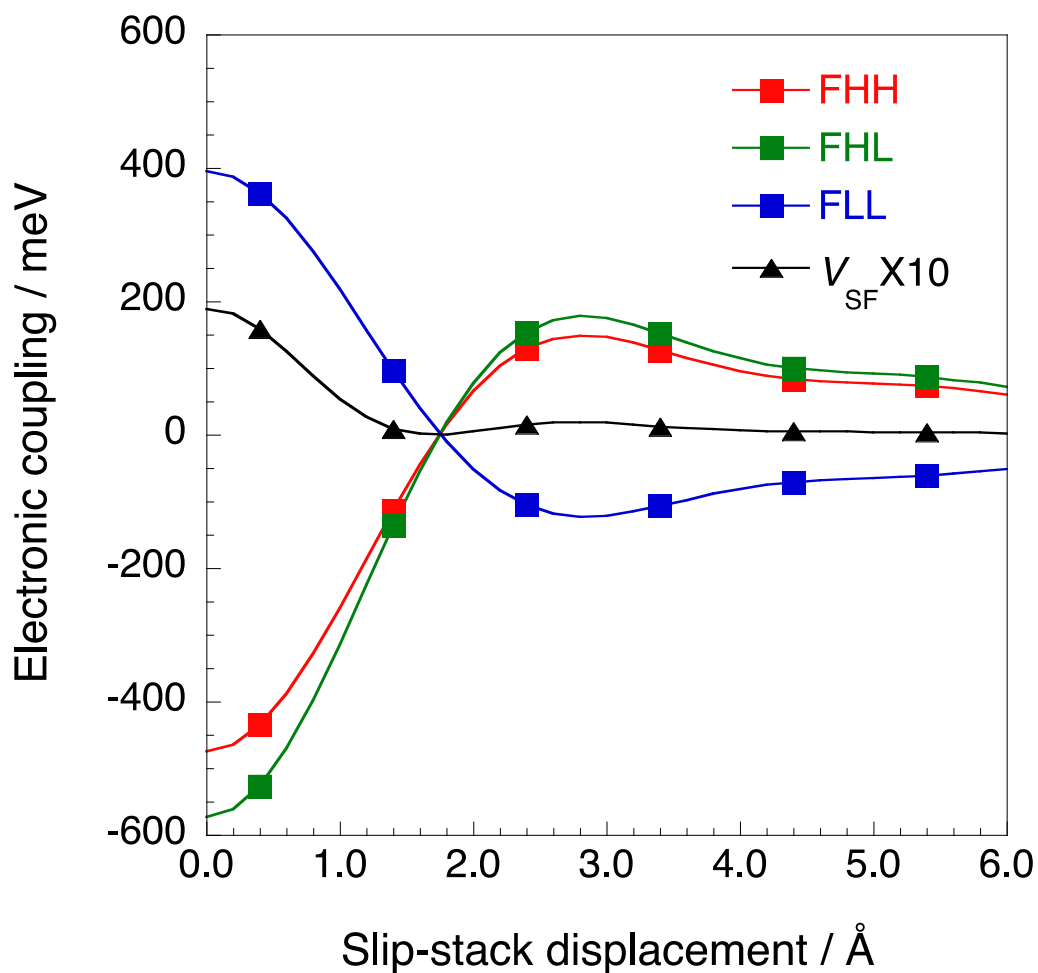


Figure S1. Fock matrix elements and SF coupling matrix element V_{SF} of $\mathbf{1}_4$ along y -axis, which is perpendicular to the x -axis considered in the text and parallel to the π -plane. Intermonomer and interdimer distances, d and D , respectively, is set to 3.0 and 3.4 Å, respectively. Note that V_{SF} is multiplied by ten.

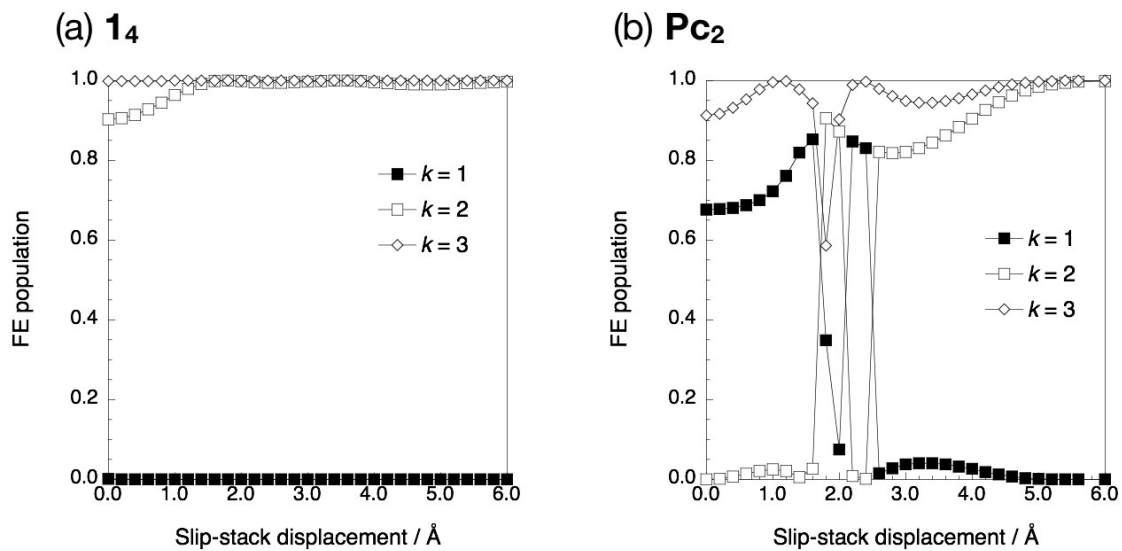


Figure S2. FE state population in low-lying eigenstates $p(\text{FE}, k)$ for $k = 1-3$ in $\mathbf{1}_4$ (a) and \mathbf{Pc}_2 (b).

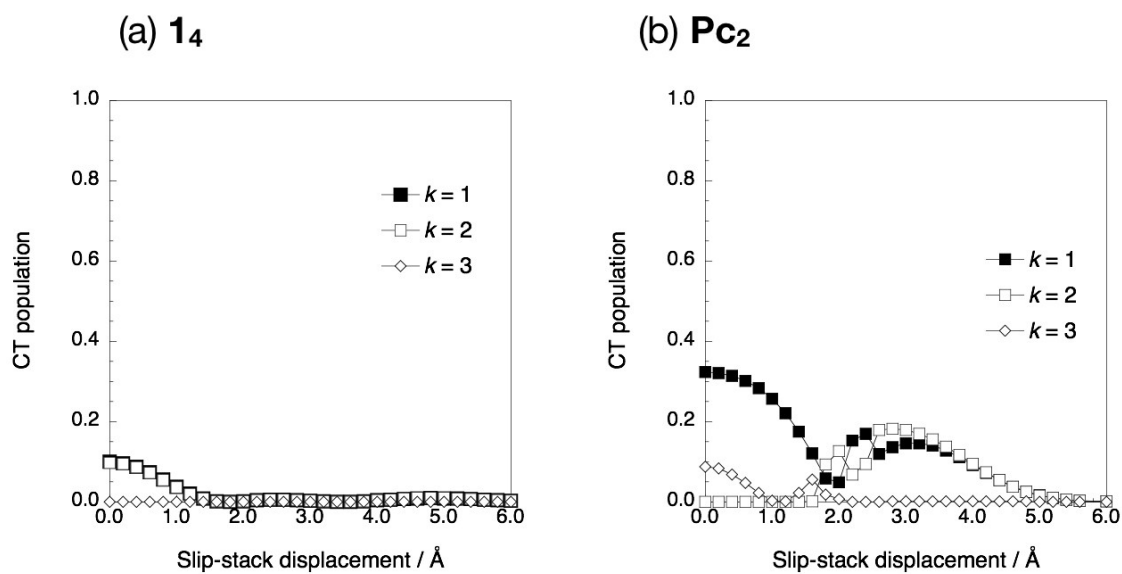


Figure S3. CT state population in low-lying eigenstates $p(\text{CT}, k)$ for $k = 1-3$ in $\mathbf{1}_4$ (a) and \mathbf{Pc}_2 (b).

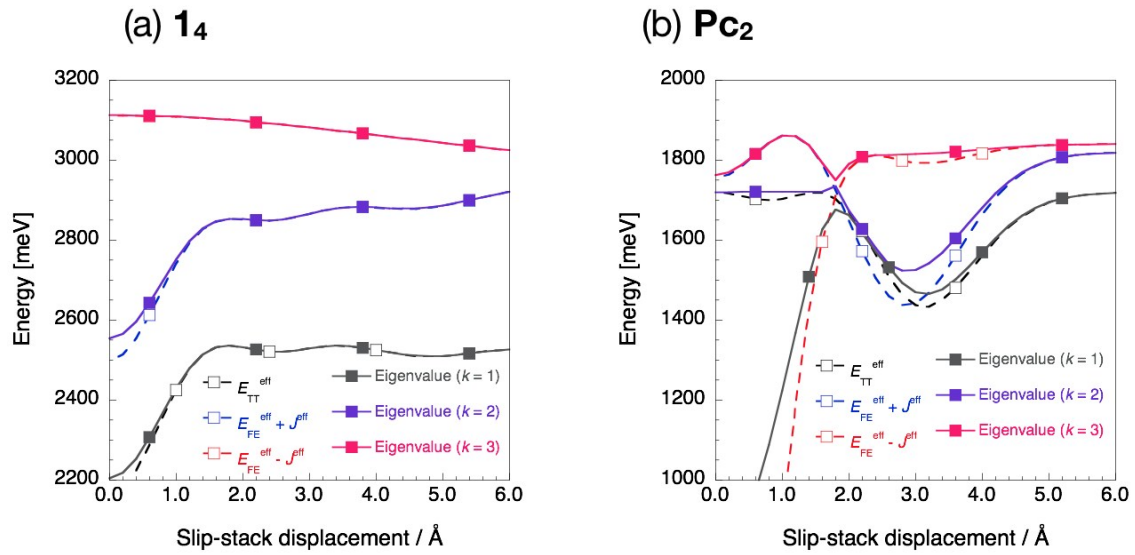


Figure S4. Comparison between the effective energies obtained from the effective Hamiltonian through the second-order quasi-degenerate perturbation theory and the eigenvalues obtained from full-diagonalization of eq 1 in the text for $\mathbf{1}_4$ (a) and for \mathbf{Pc}_2 (b). The effective energies are represented as broken lines with black for TT, blue and red for split FE states, respectively. The eigenvalues are represented as solid lines with gray for the lowest, purple for the second lowest and pink for the third lowest eigenstate, respectively.