Searching of potential energy curves for the benzene dimer using dispersion corrected density functional theory

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Fig. S1 Comparison in the potential energy curves (PEC) for parallel-displaced benzene dimer between the present theoretical results with that of counterpoise-corrected estimated CCSD(T) results of Sinnokrot et al. [M. O. Sinnokrot and C. D. Sherrill, *J. Phys. Chem. A*, 2004, 108, 10200] Here $r_1$ represents the vertical displacement while $r_2$ represents the horizontal displacement of benzene dimer.

Fig. S2 Comparison in the potential energy curves (PEC) for parallel-displaced benzene dimer between the present theoretical results with that of counterpoise-corrected MP2 results of Sinnokrot et al. [M. O. Sinnokrot and C. D. Sherrill, *J. Phys. Chem. A*, 2004, 108, 10200] Here $r_1$ represents the vertical displacement while $r_2$ represents the horizontal displacement of benzene dimer.
Supplementary information (ESI) for Physical Chemistry Chemical Physics

Interaction energy (kcal/mol)

$r_1 = 3.2 \text{ Å}$
$r_1 = 3.4 \text{ Å}$
$r_1 = 3.6 \text{ Å}$
$r_1 = 3.8 \text{ Å}$

$r_2^{PD} (\text{Å})$