Supplementary information (ESI) for *Physical Chemistry Chemical Physics*

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

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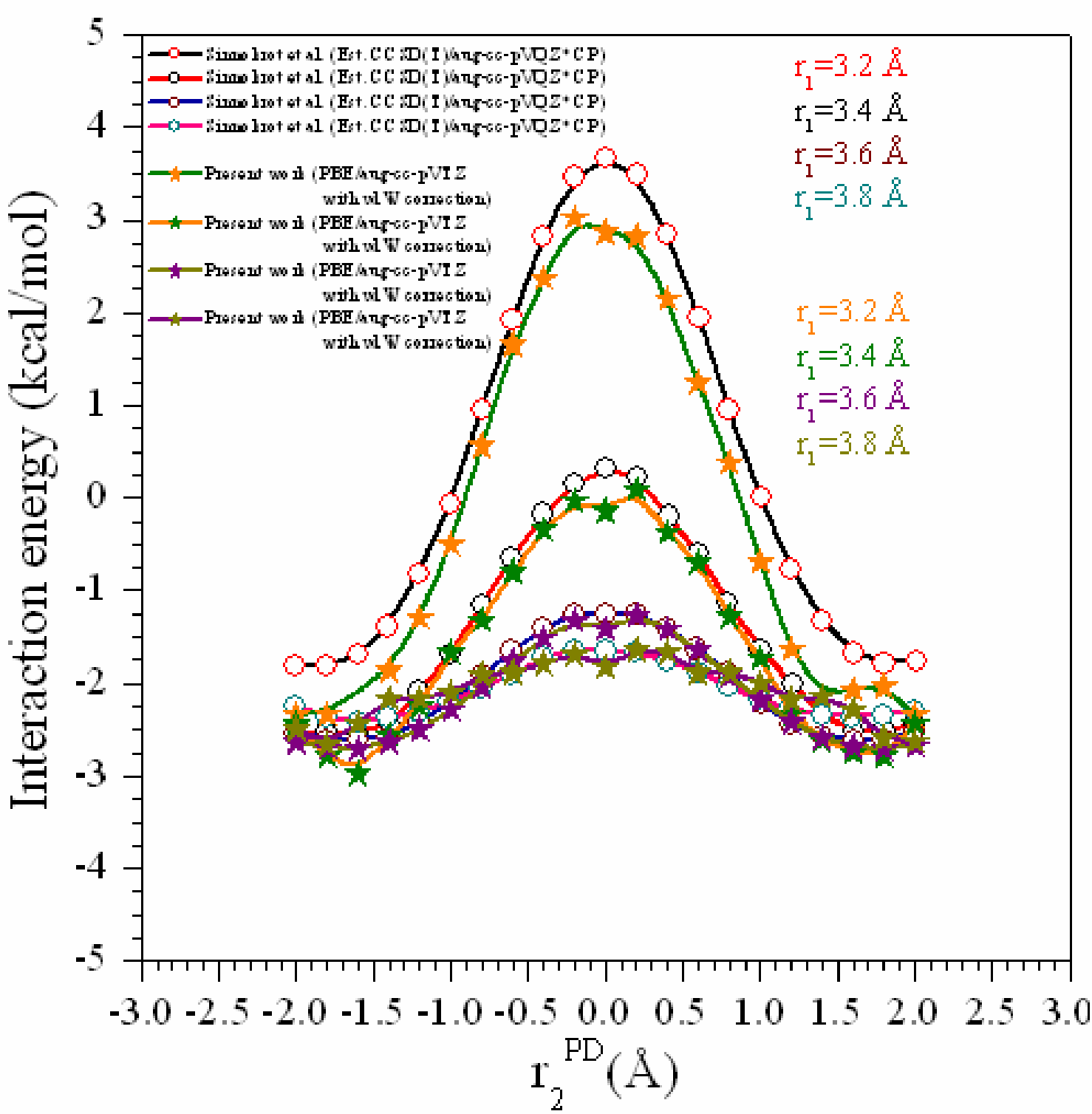
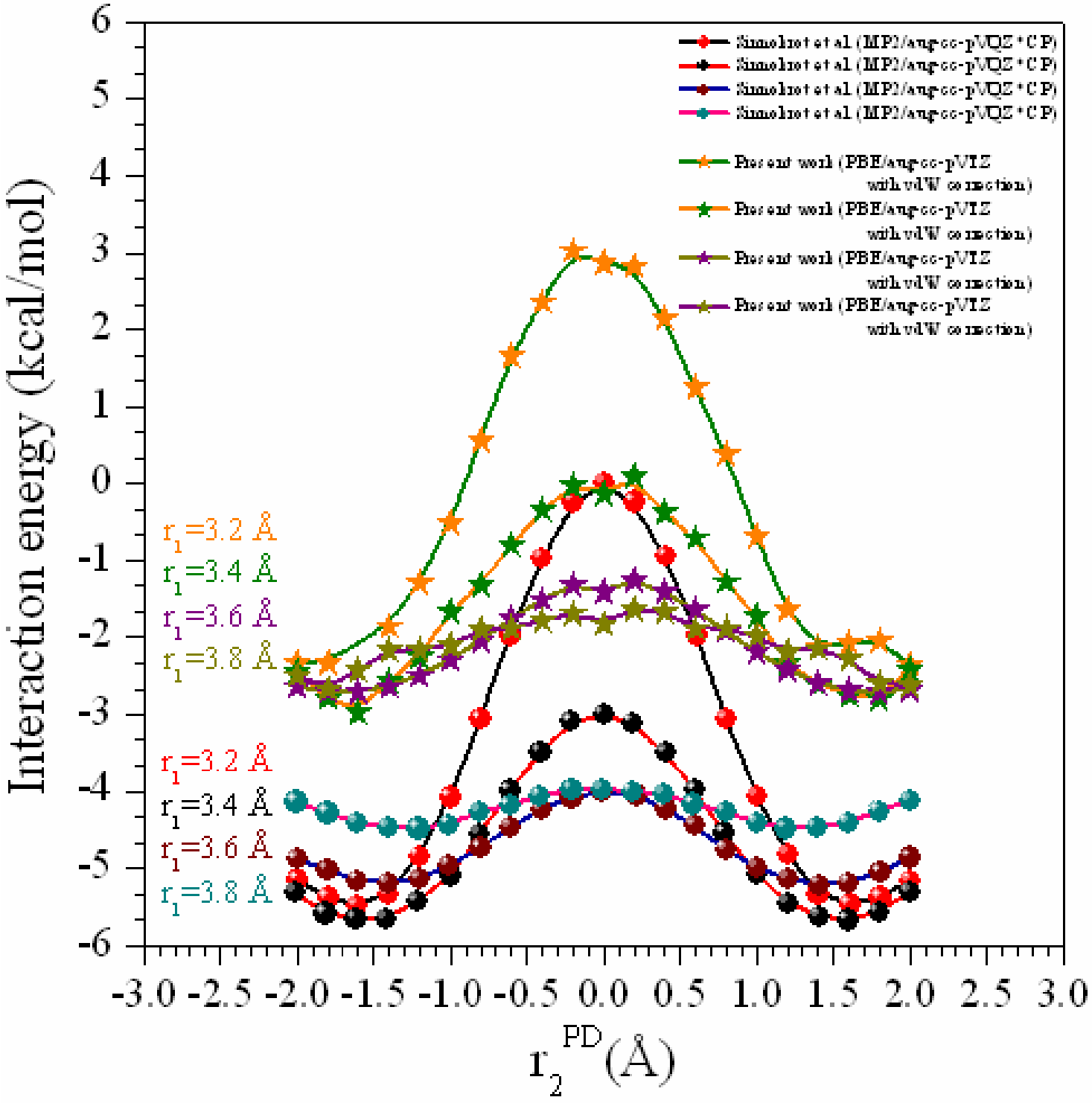
Fig. S1 Comparison in the potential energy curves (PEC) for parallel-displaced benzene dimer between the present theoretical results with that of counterpoise-corrected estimated CCSD(T) results of Sinnokrot et al.[M. O. Sinnokrot and C. D. Sherrill, *J. Phys. Chem. A*, 2004, 108, 10200] Here r_1 represents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




Simoleit et al (MP2/aug-cc-pVQZ*CP)
Simoleit et al (MP2/aug-cc-pVQZ*CP)
Simoleit et al (MP2/aug-cc-pVQZ*CP)
Simoleit et al (MP2/aug-cc-pVQZ*CP)
Present work (PBE/aug-cc-pVTZ with vdW correction)
Present work (PBE/aug-cc-pVTZ with vdW correction)
Present work (PBE/aug-cc-pVTZ with vdW correction)
Present work (PBE/aug-cc-pVTZ with vdW correction)
r1=3.2 Å
r1=3.4 Å
r1=3.6 Å
r1=3.8 Å
r1=3.2 Å
r1=3.4 Å
r1=3.6 Å
r1=3.8 Å
Interaction energy (kcal/mol)
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-3.0 -2.5 -2.0 -1.5 -1.0 -0.5 0.0 0.5 1.0 1.5 2.0 2.5 3.0
r2PD (Å)