Supplementary Information

PHENOL AND TOLUENE STACKING INTERACTIONS, INCLUDING INTERACTIONS AT LARGE HORIZONTAL DISPLACEMENTS. STUDY OF CRYSTAL STRUCTURES AND CALCULATION OF POTENTIAL ENERGY SURFACES

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The optimized phenol geometry was planar distorted hexagonal ring, with bond lengths of (O)C-C 1.394 Å, C-C 1.393 Å, O-H 0.966 Å, *ortho* C-H 1.086 Å, *meta* C-H 1.084 Å and *para* C-H 1.083 Å. The optimized toluene geometry was also planar distorted hexagonal ring, with bond lengths of (C)C-C 1.397 Å, C-C 1.393 Å, C-H 1.093Å, *ortho* C-H 1.086 Å, *meta* C-H 1.084 Å and *para* C-H 1.084 Å.

The minimum of interaction energy of two parallel phenol molecule at the r= 0.0 Å and R= 3.8 Å is -1.67 kcal/mol.

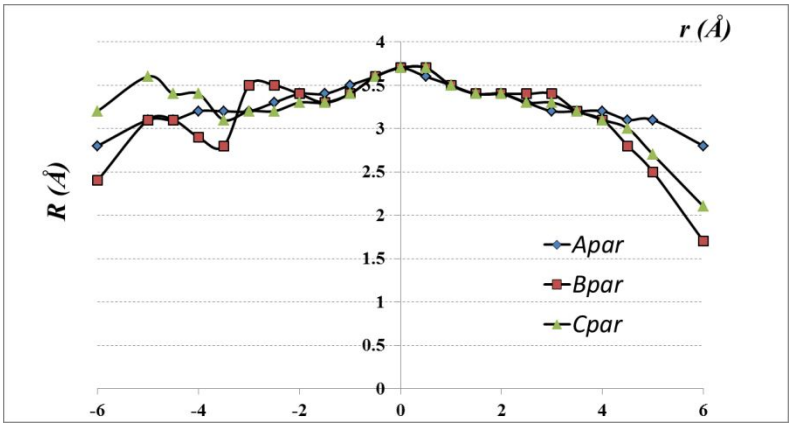

Figure SI 1. The optimal normal distances (R) for three different parallel orientations of phenol-phenol molecules plotted as a function of the r value. The A_{par}, B_{par} and C_{par} orientations are presented in **Figure 13**.

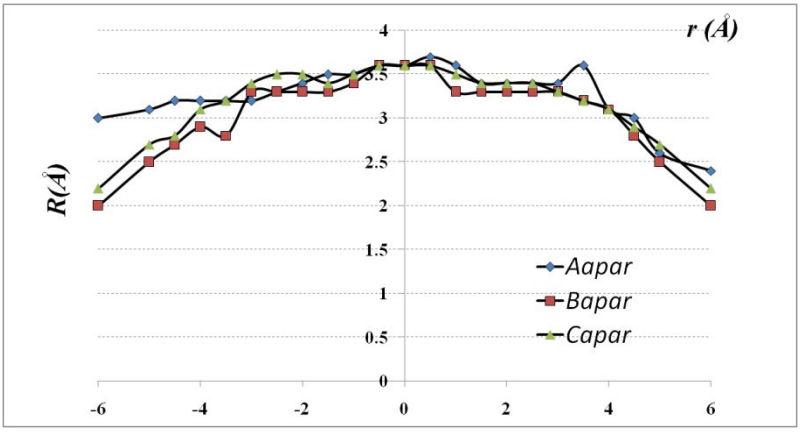

Figure SI 2. The optimal normal distances (R) for three different antiparallel orientations of phenol-phenol molecules plotted as a function of the r value. The A_{apar}, B_{apar} and C_{apar} orientations are presented in **Figure 14**.

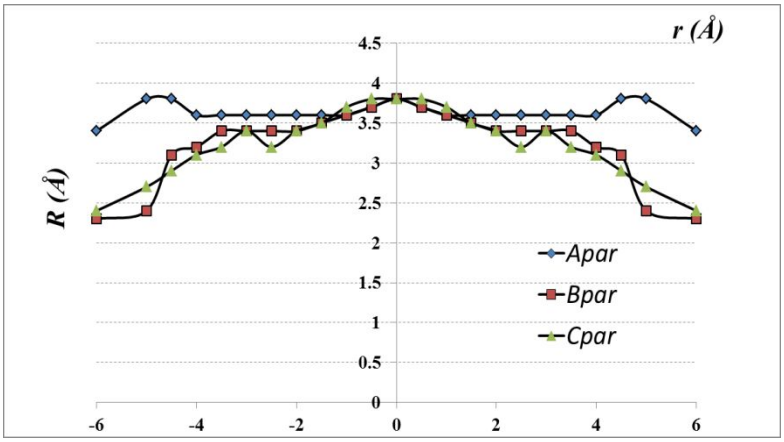

Figure SI 3. The optimal normal distances (R) for three different parallel orientations of toluene-toluene molecules plotted as a function of the r value. The A_{par}, B_{par} and C_{par} orientations are presented in **Figure 18**.

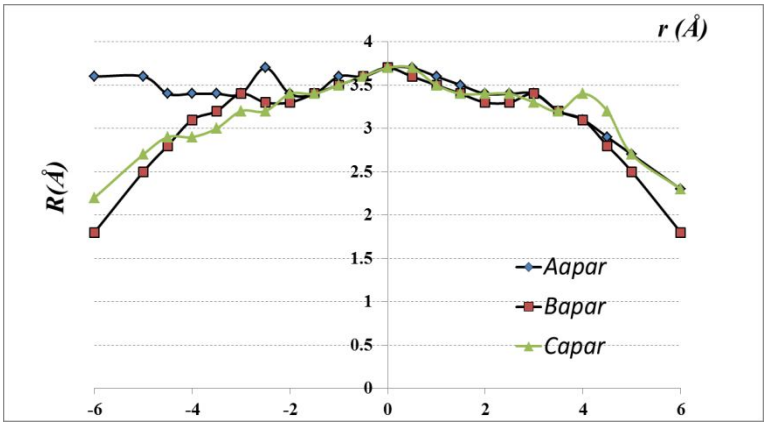

Figure SI 4. The optimal normal distances (R) for three different parallel orientations of toluene-toluene molecules plotted as a function of the r value. The A_{apar}, B_{apar} and C_{apar} orientations are presented in **Figure 19**.