

Supplementary material to "Structures and interaction energies of stacked graphene-nucleobase complexes"

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FIG. S1: B97-D/TZV(d,p) three dimensional potential energy surface of adenine on $C_{96}H_{24}$. The structure corresponds to the origin of the plot. Axis labels in \AA , contour levels in kcal/mol.

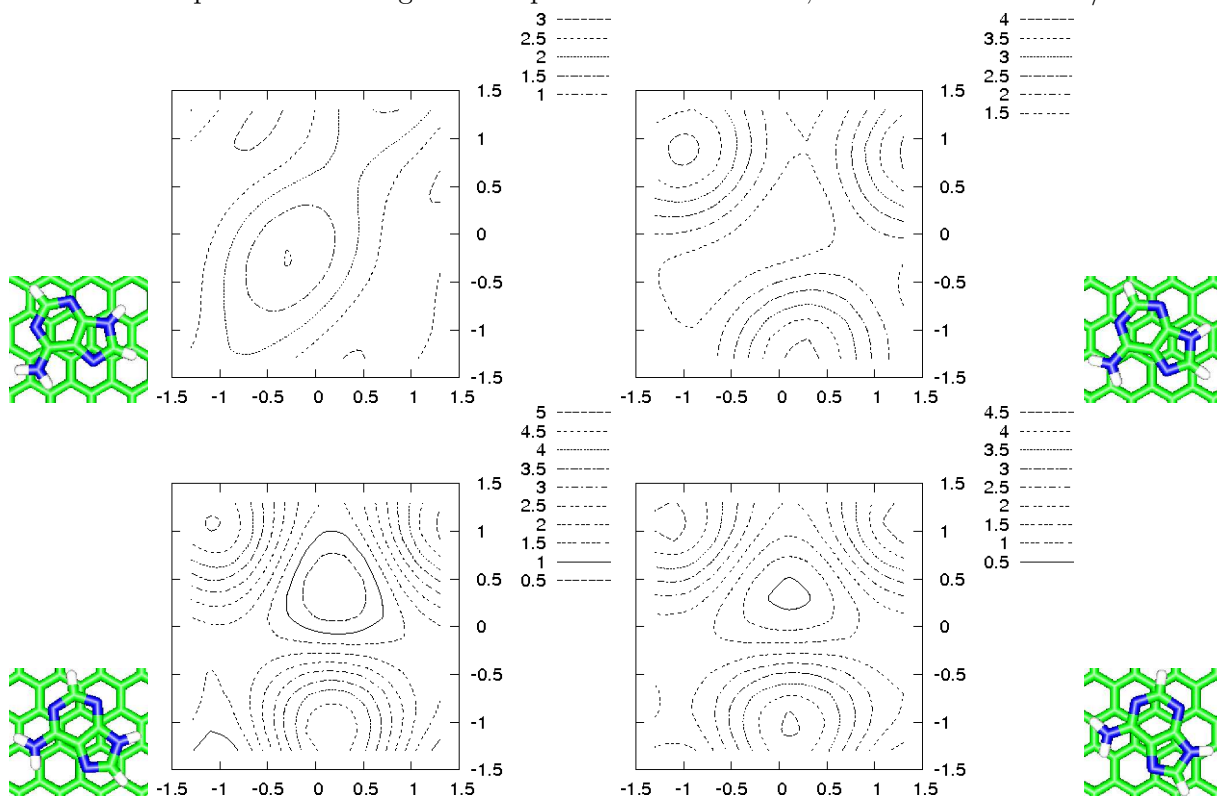


FIG. S2: B97-D/TZV(d,p) three dimensional potential energy surface of thymine on $C_{96}H_{24}$.

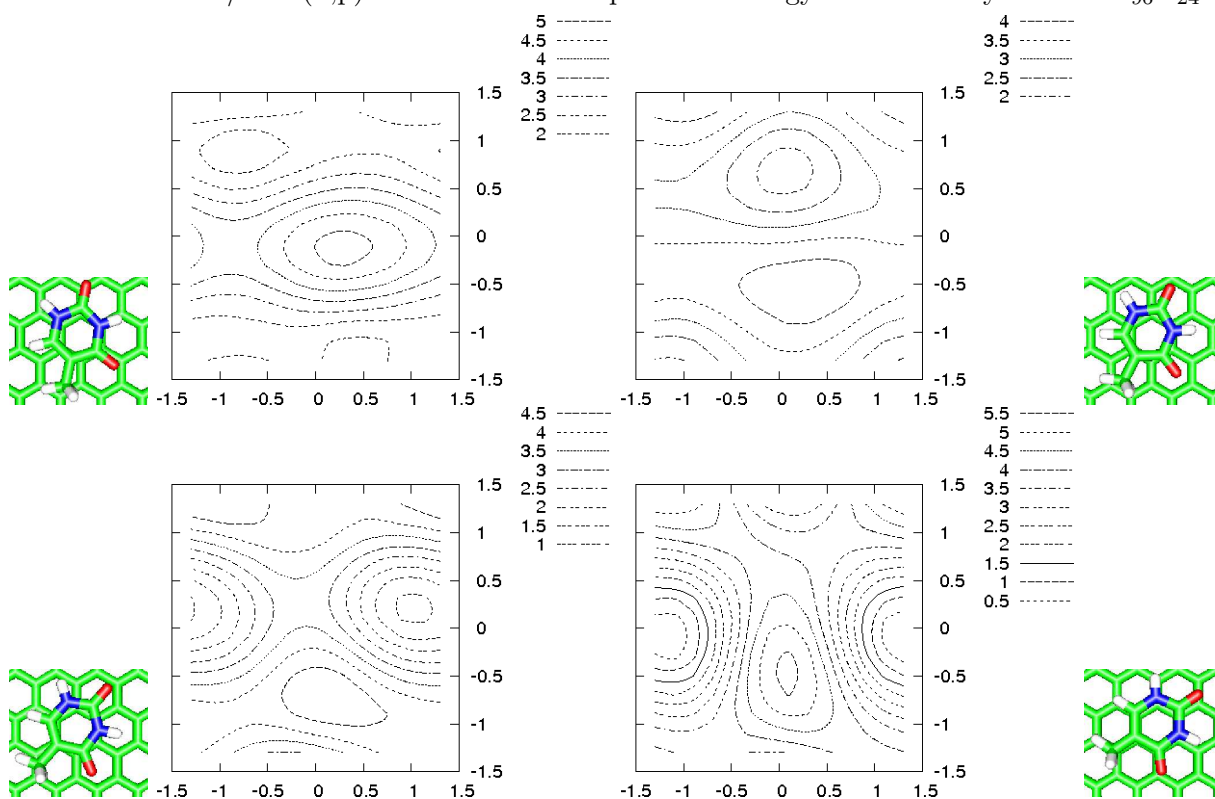


FIG. S3: B97-D/TZV(d,p) three dimensional potential energy surface of cytosine on $C_{96}H_{24}$.

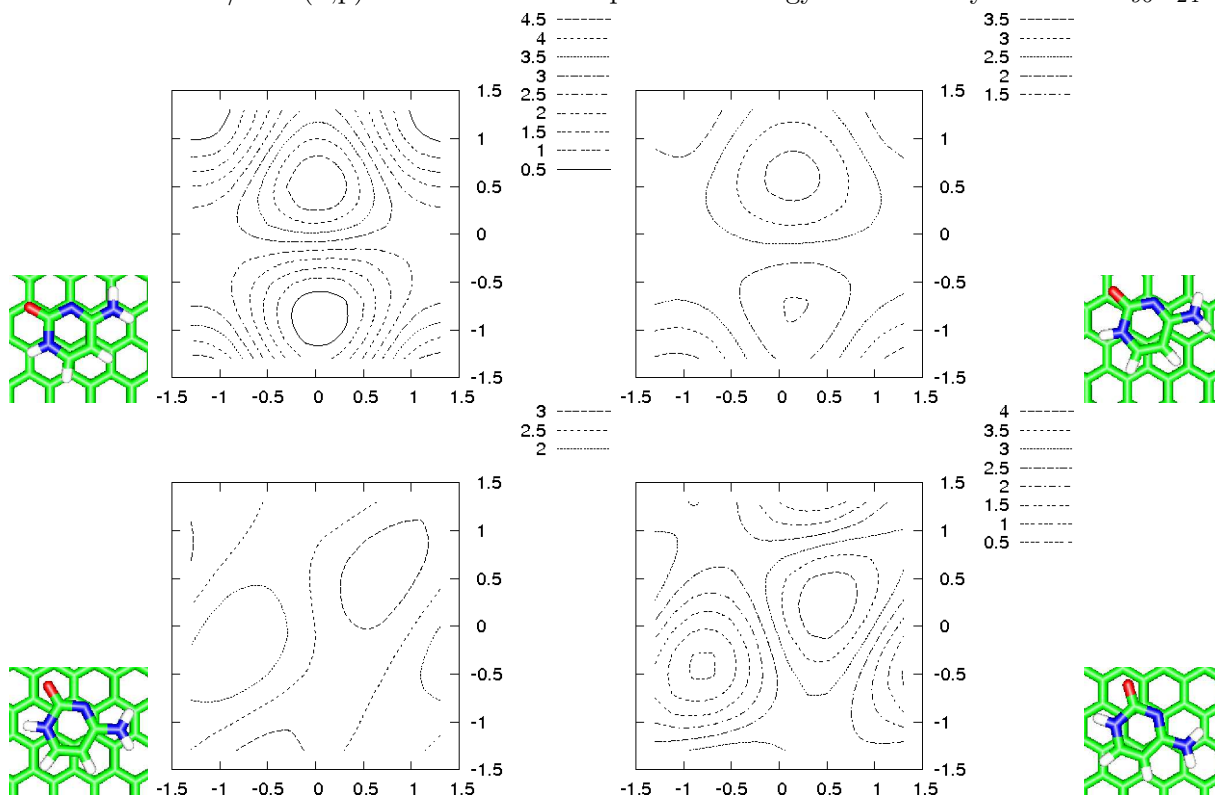


FIG. S4: B97-D/TZV(d,p) three dimensional potential energy surface of guanine on $C_{96}H_{24}$.

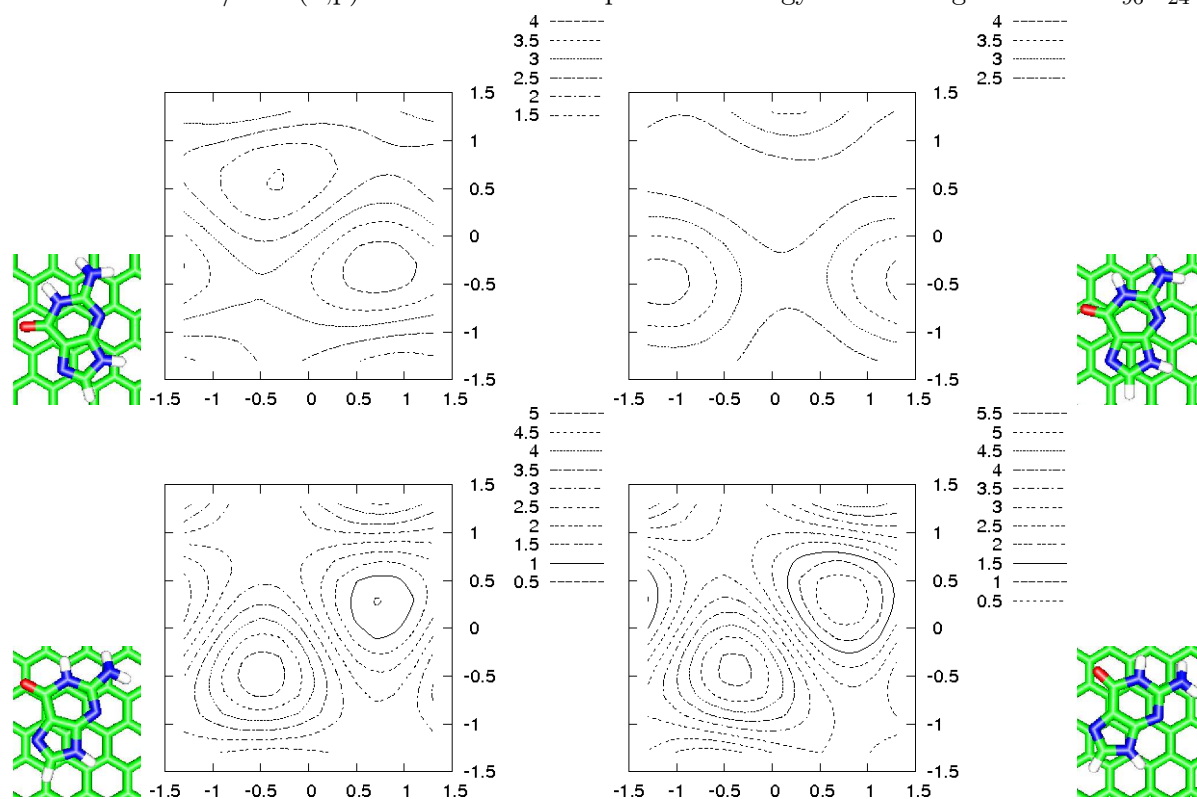


FIG. S5: B97-D/TZV(d,p) three dimensional potential energy surface of uracil on $C_{96}H_{24}$.

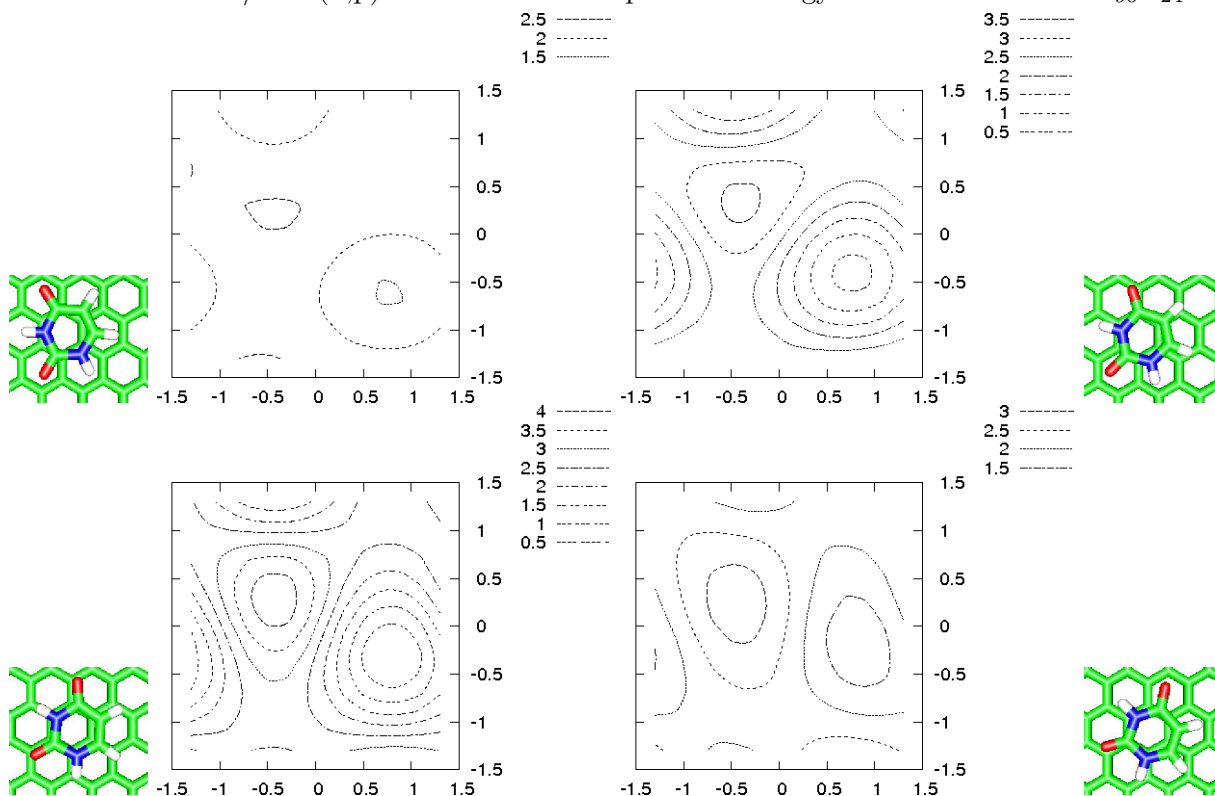


FIG. S6: Intermolecular interaction energies of adenine ... graphene sheet complexes with different size. n is the number of the carbon atoms in the sheet.

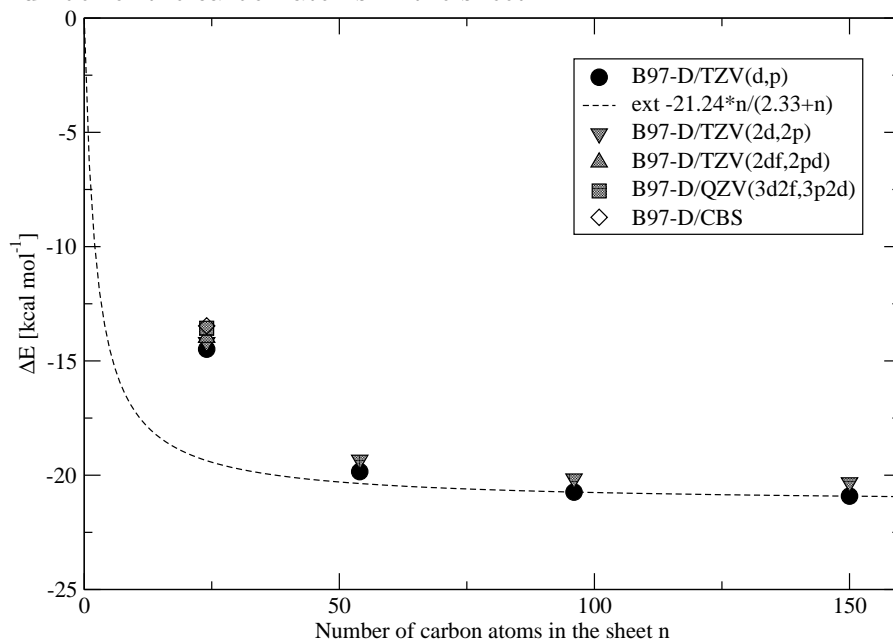


FIG. S7: Intermolecular interaction energies of thymine ... graphene sheet complexes with different size.

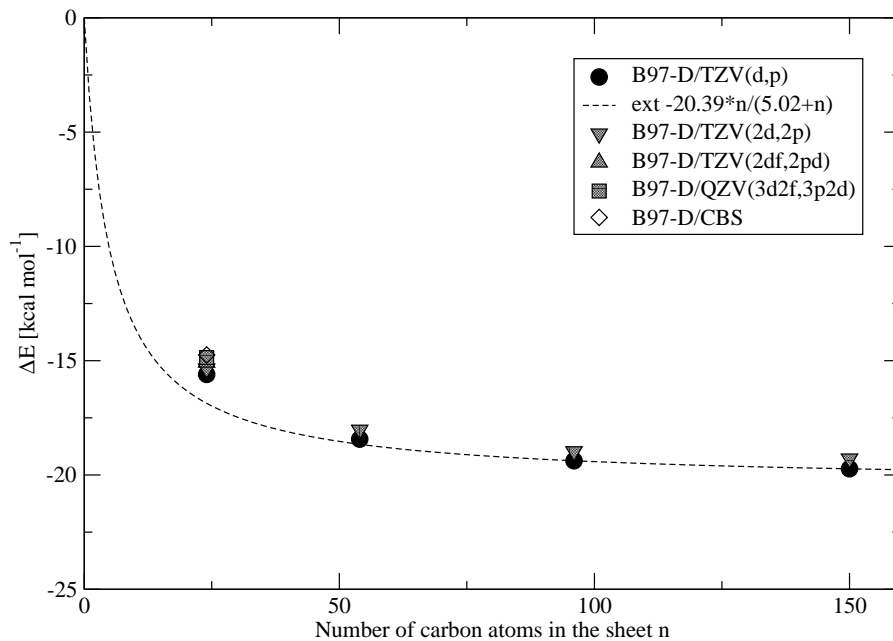


FIG. S8: Intermolecular interaction energies of cytosine ... graphene sheet complexes with different size.

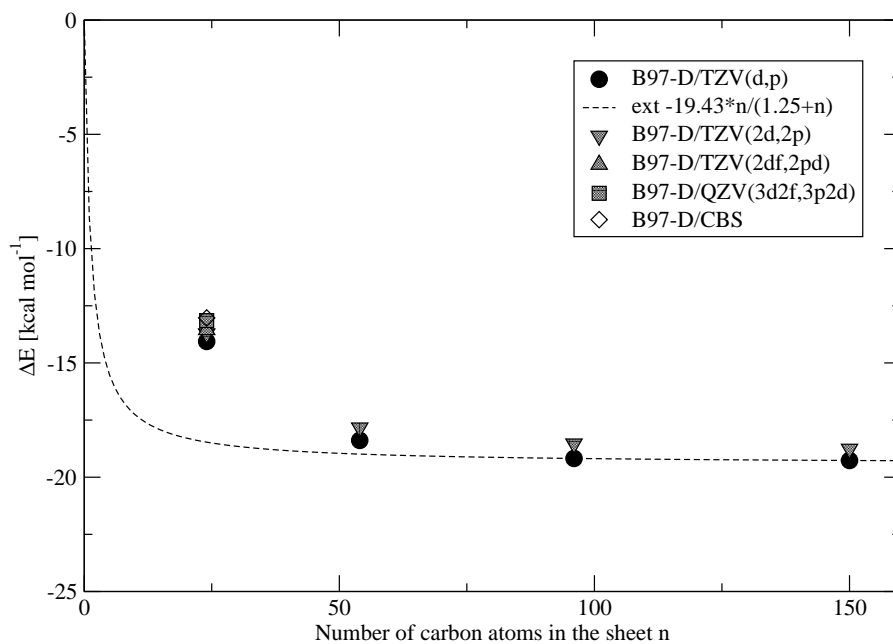


FIG. S9: Intermolecular interaction energies of guanine ... graphene sheet complexes with different size.

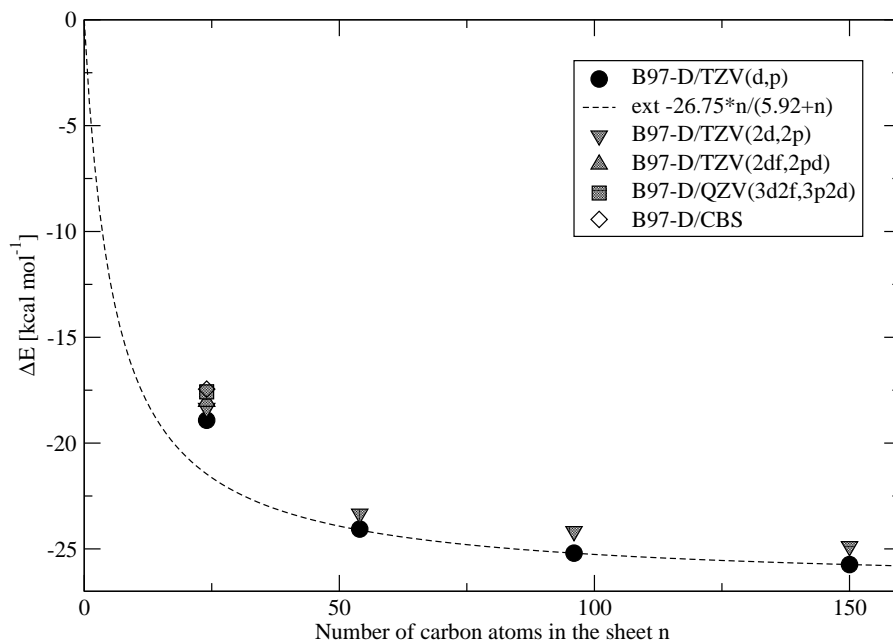


FIG. S10: Intermolecular interaction energies of uracil ... graphene sheet complexes with different size.

