Supporting information:

Observation and analysis of small inclination of thymine molecules on graphite

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1. Dimer calculation result

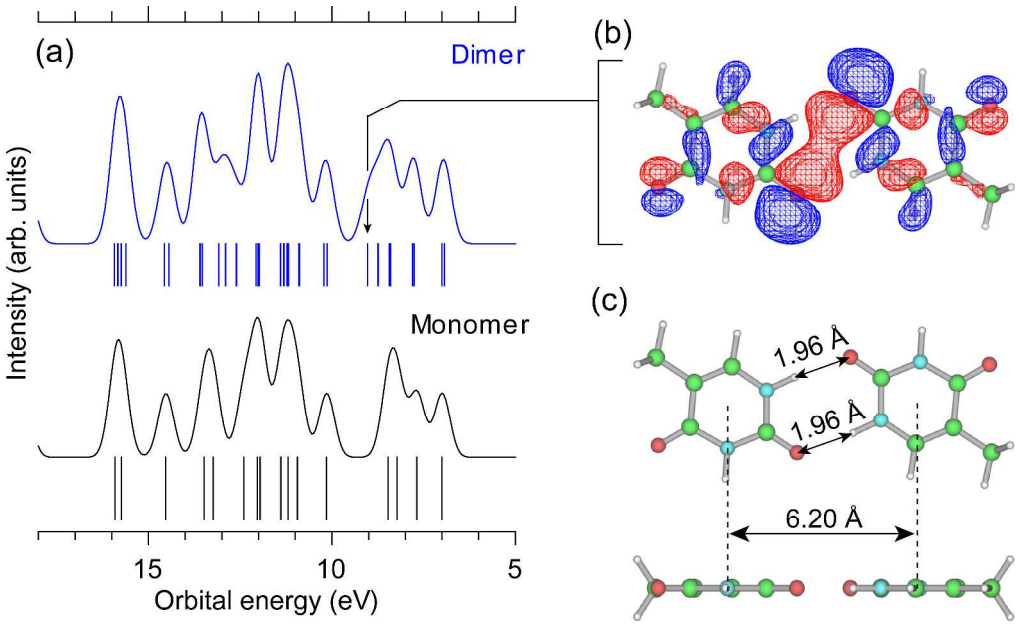

Fig. S1: (a) Calculated DOS and MO energies of thymine monomer and dimer obtained using the Gaussian 03W package with the B3LYP/6-311++G** basis set. The monomer spectrum is the same as shown in Fig. 3 in the main text. (b) A schematic of a spatial distributions of hybridized O(2p) orbital between two molecules in the dimer, which is not seen in the monomer structure. (c) Top and side views of the dimer structure. The structure used here was obtained by optimization of the dimer adsorbed on a graphite surface by Komiyama, et al. [see Ref. "Komiyama, M.; Uchihashi, T.; Sugawara, Y.; Morita, S.; Surf. Interface Anal. **2001**, 32, 53-56"].