Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

DFT Study on the Interaction between Glycine Molecules/Radicals with (8, 0) SiCNT

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Supporting Information

Figure S1. The band structures of individual glycine molecule adsorbed on (8, 0) SiCNT with the (a) monodentate configurations for *trans*-I and *cis*-II; (b) cycloaddition configurations for *trans*-I and *cis*-II as well as dissociation configurations for *trans*-I. The Fermi level is dotted with a red line.

Figure S2. The optimized configurations of maximum number of glycine molecules adsorbed on the (n, 0) (n=7, 8, 9 and10) SiCNTs based on the configuration of M_I-a.

Figure S3. The plotted HOMO and LUMO of glycine radicals adsorbed on (8, 0) SiCNT with isosurface values of 0.03 a.u.

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Supporting information

Figure S1(a).

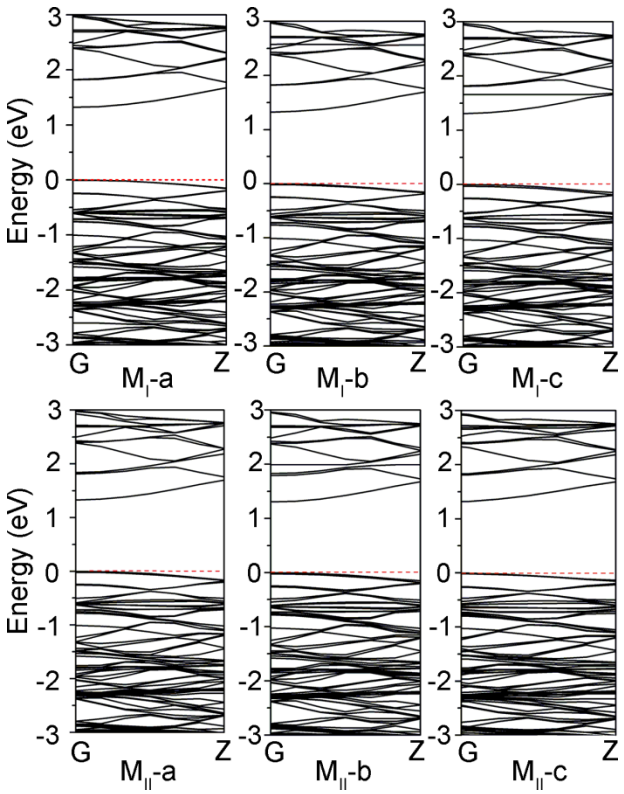

Figure S1(b).

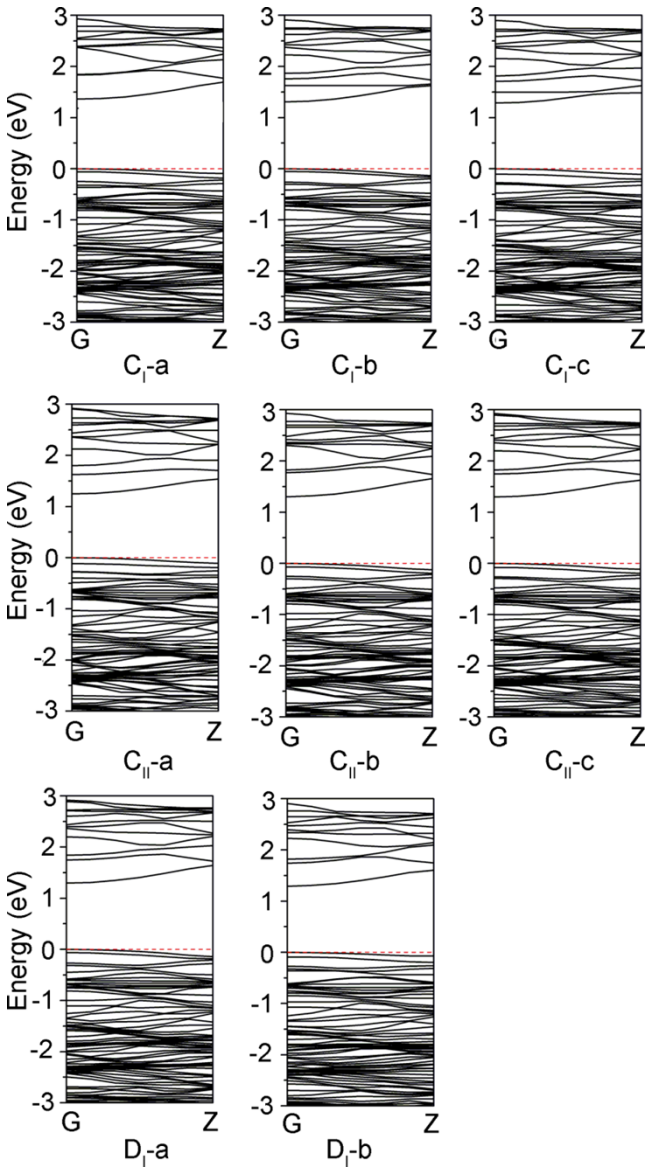

Figure S2.

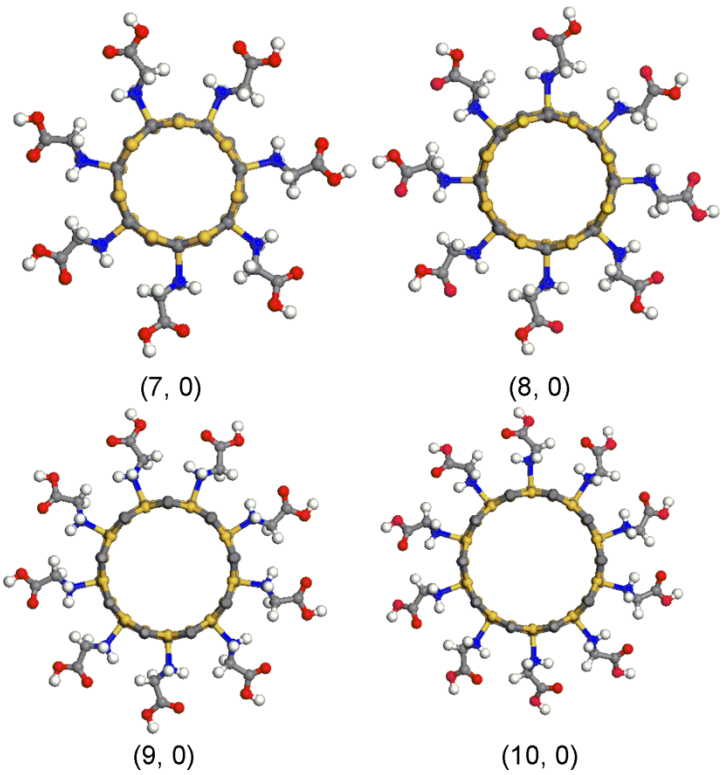

Figure S3.