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The Supporting Information of "Insights into the Adsorption Mechanism and Dynamic Behavior of Tetracycline Antibiotics on Reduce Graphene Oxide (RGO) and Graphene Oxide (GO) Materials"

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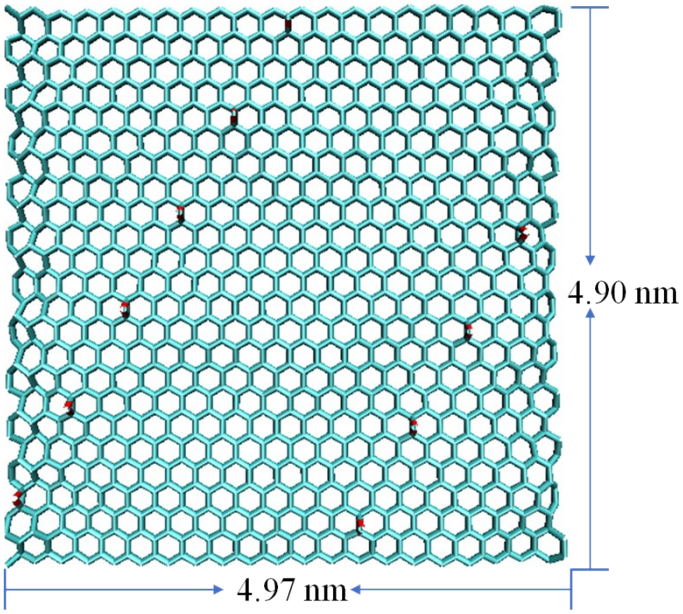

Figure S1. The GO model used in molecular dynamics simulations

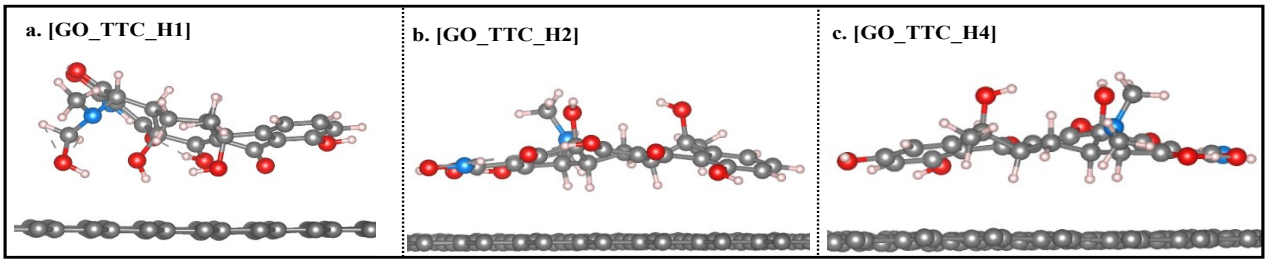

Figure S2. The optimized geometries of partial GO_TTC complexes, bonds are in Å.

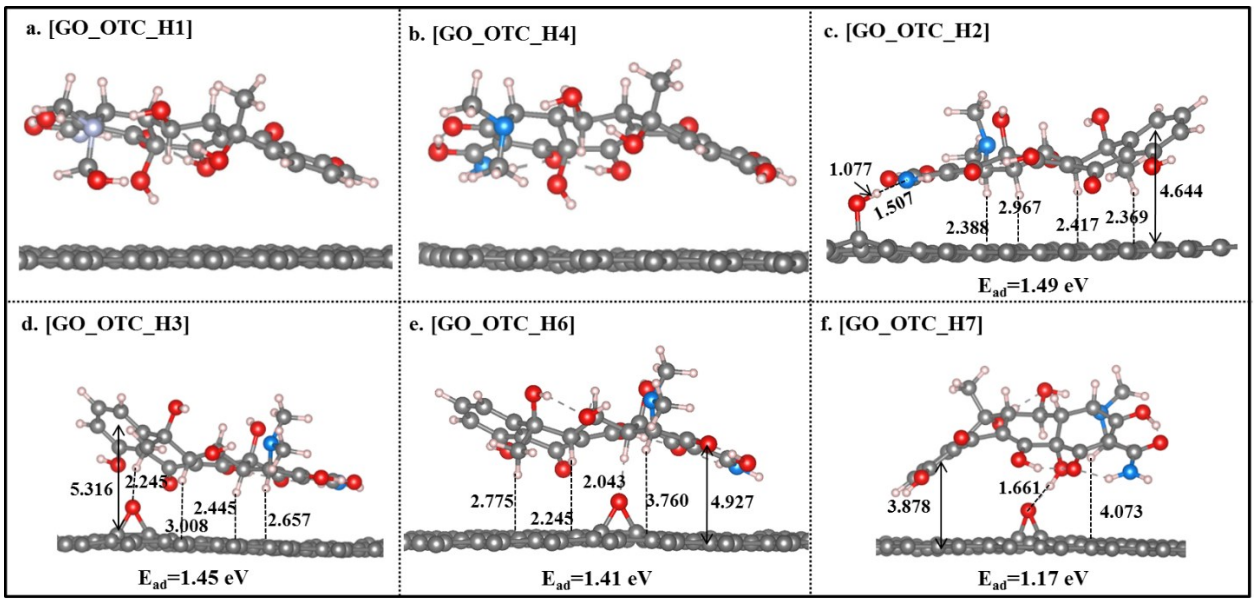

Figure S3. The optimized geometries of partial GO_OTC complexes, bonds are in Å.

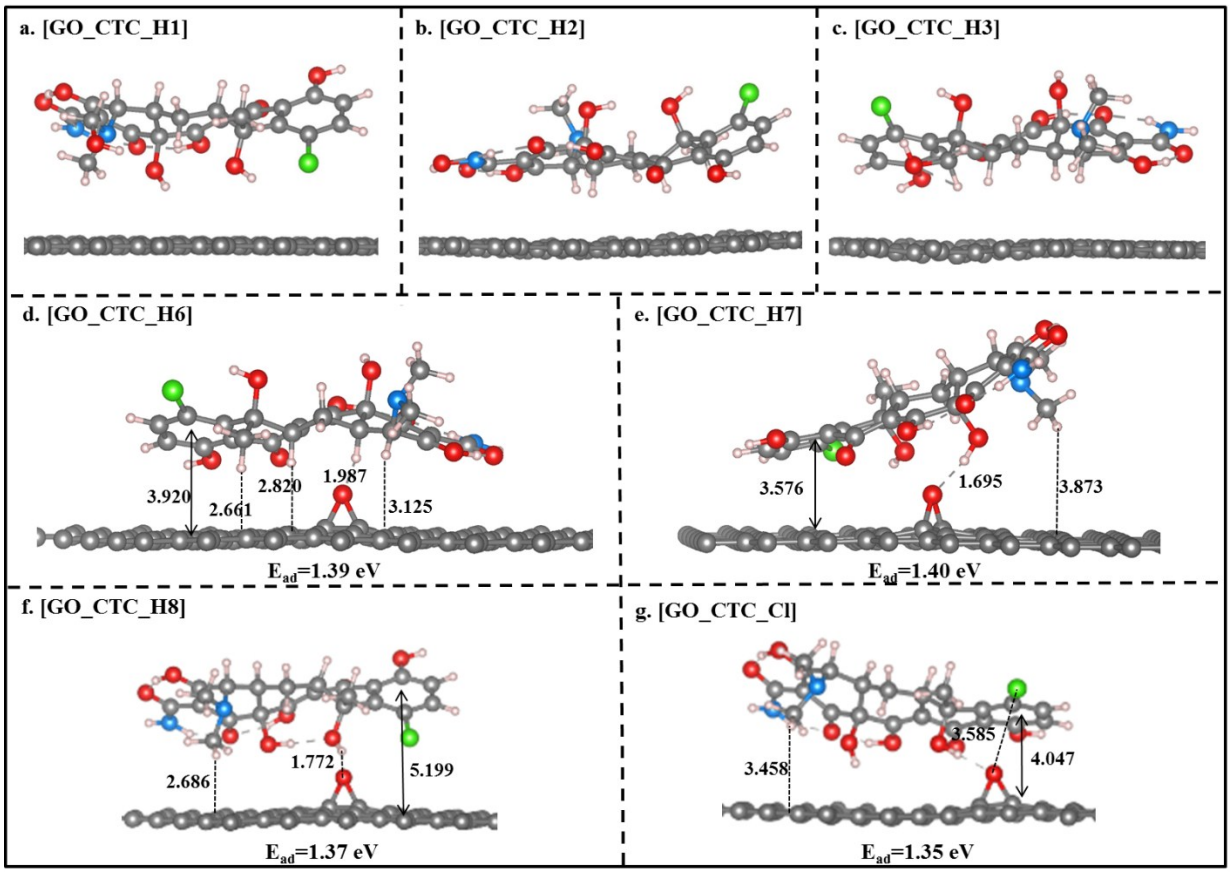

Figure S4. The optimized geometries of partial GO_CTC complexes, bonds are in Å.

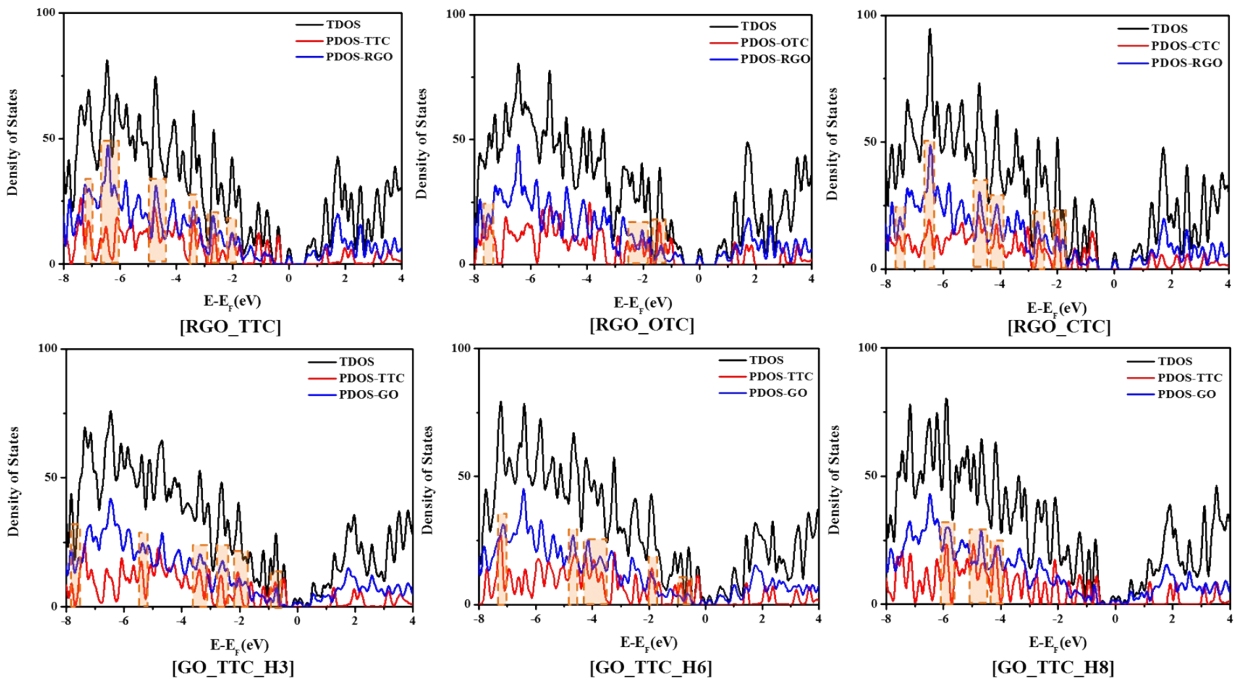

Figure S5. The density of states of RGO_TCs systems and partial GO_TTC systems.

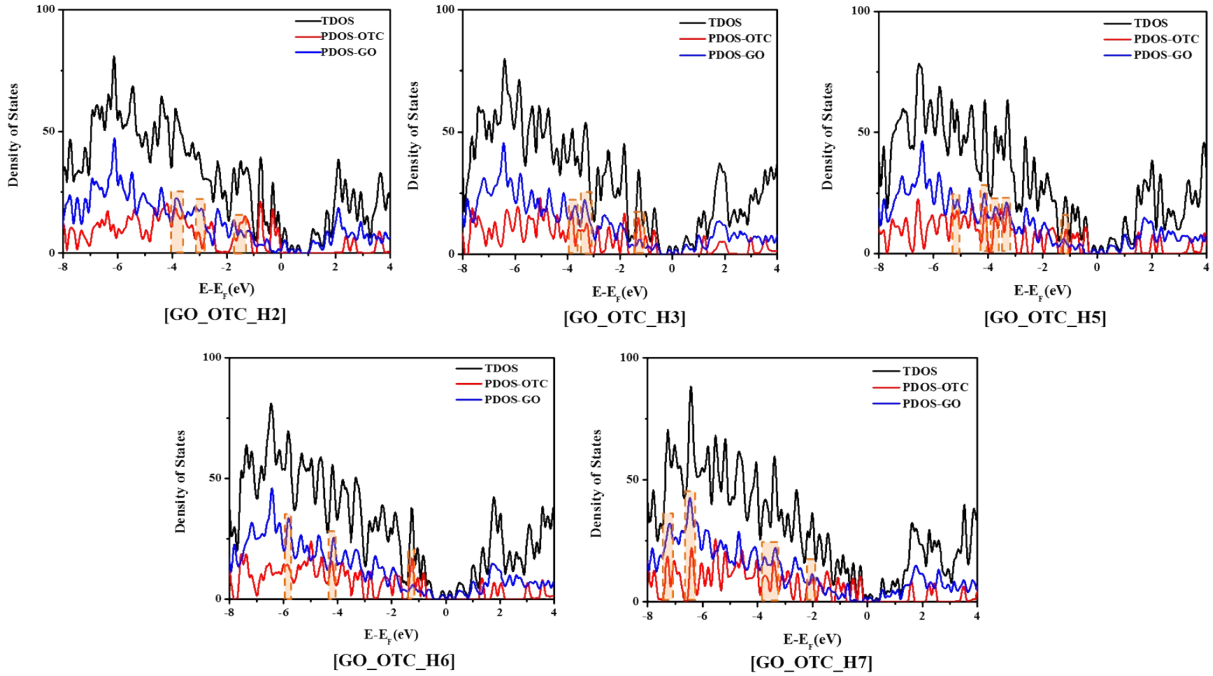

Figure S6. The density of states of GO_OTC systems.

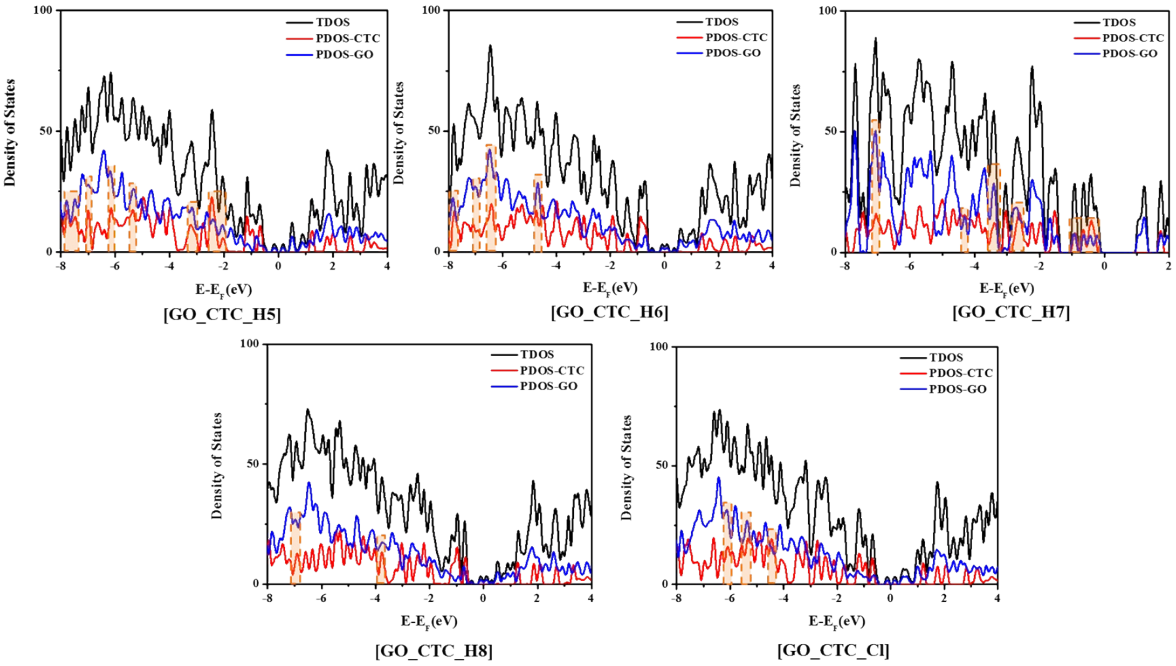

Figure S7. The density of states of GO_CTC systems.

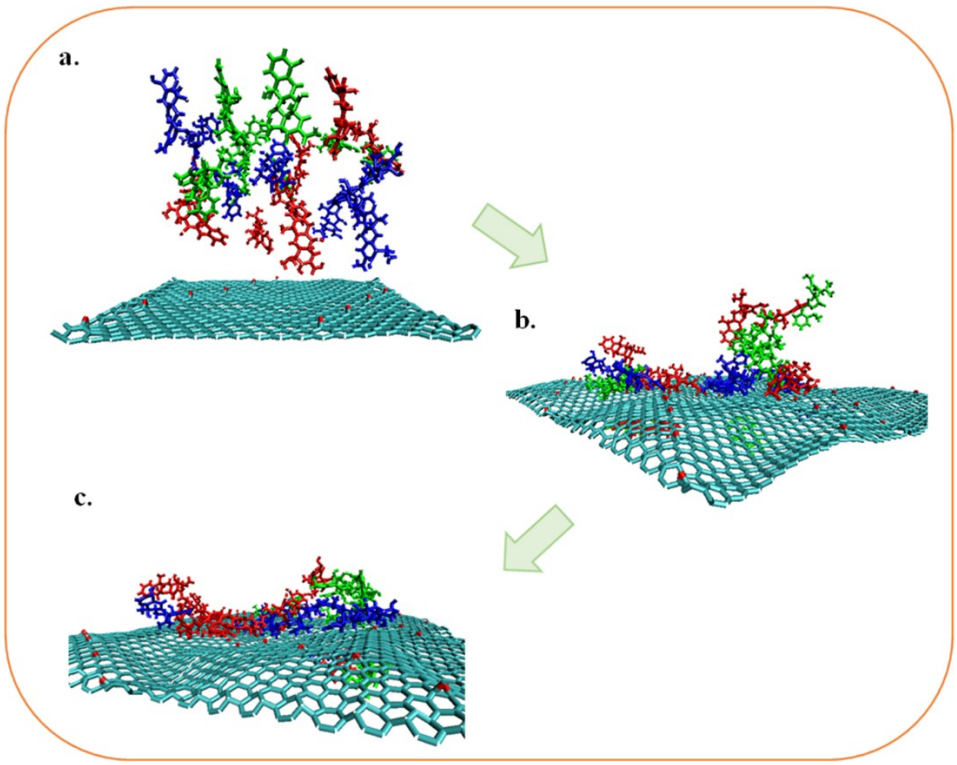

Figure S8. Snapshots from MD simulations which show the changes of TCs at the surface of GO. (Color code: TTC, red; OTC, green; CTC, blue; GO-C atoms, cyan; GO-O atoms, red.)

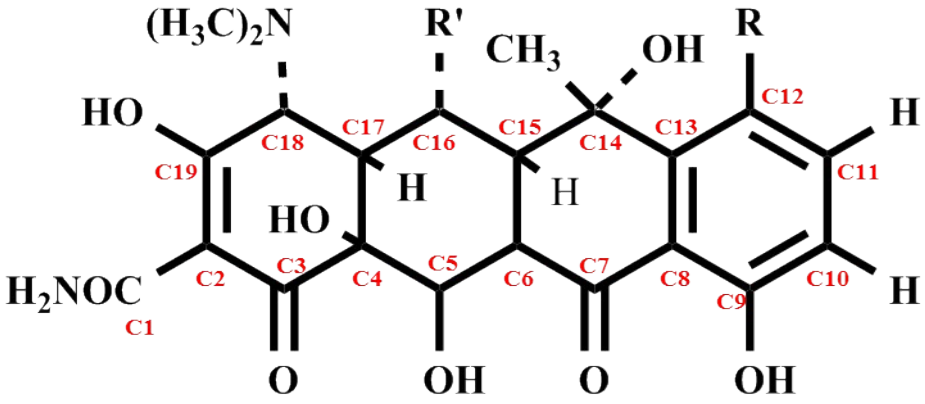

Figure S9. The scheme of TCs with C labels.

Table S1. The ESP values of the active sites of TCs

TTC	ESP value (kcal/mol)	OTC	ESP value (kcal/mol)	CTC	ESP value (kcal/mol)
H1	14.72	H1	13.04	H1	13.35
H2	52.11	H2	52.11	H2	51.09
H3	19.32	H3	1.89	H3	14.23
H4	19.63	H4	16.92	H4	24.75

H5	56.27	H5	57.18	H5	63.26
H6	31.47	H6	30.31	H6	29.02
H7	48.99	H7	50.10	H7	47.57
H8	40.51	H8		H8	29.02
Cl		Cl		Cl	9.40

Table S2. The bond lengths changes of in carbon rings of TTC before and after adsorption on RGO and GO. The labels of C were shown in Fig. S9

	TTC	RGO_TTC	GO_TTC_H3	GO_TTC_H5	GO_TTC_H6	GO_TTC_H7	GO_TTC_H7
C1-C2	1.469	1.473	1.475	1.470	1.473	1.473	1.472
C2-C3	1.438	1.437	1.437	1.438	1.440	1.438	1.440
C3-C4	1.549	1.554	1.549	1.549	1.551	1.544	1.551
C4-C5	1.532	1.532	1.536	1.524	1.533	1.540	1.530
C5-C6	1.365	1.368	1.367	1.362	1.370	1.375	1.363
C6-C7	1.486	1.485	1.488	1.485	1.484	1.477	1.487
C7-C8	1.501	1.501	1.501	1.494	1.478	1.499	1.502
C8-C9	1.412	1.418	1.419	1.413	1.417	1.415	1.408
C9-C10	1.402	1.400	1.402	1.403	1.400	1.410	1.402
C10-C11	1.390	1.387	1.386	1.389	1.388	1.390	1.391
C11-C12	1.396	1.394	1.396	1.398	1.395	1.395	1.398
C12-C13	1.395	1.396	1.394	1.395	1.397	1.397	1.394
C13-C14	1.523	1.526	1.525	1.524	1.525	1.532	1.525
C14-C15	1.558	1.557	1.555	1.558	1.556	1.555	1.560
C15-C16	1.528	1.531	1.529	1.529	1.531	1.531	1.531
C16-C17	1.518	1.516	1.517	1.519	1.515	1.520	1.521
C17-C18	1.538	1.546	1.546	1.549	1.536	1.548	1.537
C18-C19	1.507	1.504	1.505	1.506	1.499	1.505	1.504
C19-C2	1.417	1.413	1.411	1.411	1.413	1.410	1.414
C4-C17	1.524	1.521	1.526	1.522	1.517	1.524	1.523
C6-C15	1.521	1.517	1.516	1.521	1.523	1.524	1.524
C8-C13	1.411	1.416	1.419	1.410	1.412	1.413	1.411

Table S3. The bond lengths changes of in carbon rings of OTC before and after adsorption on RGO and GO. The labels of C were shown in Fig. S9

	OTC	RGO	GO_OTC_H2	GO_OTC_H3	GO_OTC_H5	GO_OTC_H6	GO_OTC_H7
C1-C2	1.459	1.454	1.489	1.466	1.459	1.465	1.47
C2-C3	1.439	1.436	1.426	1.436	1.437	1.438	1.437
C3-C4	1.546	1.544	1.549	1.543	1.542	1.549	1.539
C4-C5	1.522	1.522	1.533	1.527	1.521	1.529	1.539
C5-C6	1.353	1.355	1.366	1.364	1.352	1.361	1.36
C6-C7	1.495	1.491	1.482	1.489	1.493	1.489	1.487
C7-C8	1.487	1.487	1.489	1.486	1.484	1.487	1.494
C8-C9	1.419	1.422	1.424	1.424	1.421	1.422	1.419
C9-C10	1.398	1.396	1.398	1.397	1.401	1.398	1.398
C10-C11	1.391	1.391	1.391	1.391	1.39	1.391	1.391
C11-C12	1.393	1.391	1.393	1.391	1.395	1.392	1.393
C12-C13	1.398	1.399	1.397	1.397	1.397	1.398	1.398
C13-C14	1.522	1.525	1.522	1.524	1.522	1.521	1.52
C14-C15	1.586	1.579	1.578	1.578	1.588	1.575	1.585
C15-C16	1.522	1.525	1.525	1.527	1.522	1.527	1.521
C16-C17	1.533	1.54	1.537	1.537	1.54	1.533	1.538
C17-C18	1.553	1.56	1.549	1.553	1.556	1.537	1.553
C18-C19	1.518	1.524	1.533	1.513	1.521	1.516	1.516
C19-C2	1.421	1.423	1.432	1.413	1.421	1.421	1.412
C4-C17	1.529	1.531	1.526	1.531	1.531	1.517	1.534
C6-C15	1.51	1.51	1.51	1.513	1.506	1.514	1.508
C8-C13	1.414	1.412	1.416	1.413	1.414	1.413	1.413

Table S4. The bond lengths changes of in carbon rings of OTC before and after adsorption on RGO and GO. The labels of C were shown in Fig. S9

	CTC	RGO_CTC	GO_CTC_H5	GO_CTC_H6	GO_CTC_H7	GO_CTC_H8	GO_CTC_Cl
C1-C2	1.475	1.472	1.471	1.474	1.474	1.471	1.473
C2-C3	1.438	1.434	1.43	1.439	1.438	1.44	1.436
C3-C4	1.552	1.547	1.549	1.553	1.545	1.547	1.547
C4-C5	1.533	1.534	1.541	1.525	1.539	1.544	1.533
C5-C6	1.366	1.371	1.37	1.36	1.374	1.366	1.372
C6-C7	1.473	1.465	1.473	1.475	1.459	1.464	1.471
C7-C8	1.512	1.511	1.51	1.501	1.511	1.514	1.507

C8-C9	1.419	1.42	1.425	1.424	1.418	1.413	1.418
C9-C10	1.398	1.397	1.402	1.398	1.396	1.399	1.398
C10-C11	1.387	1.386	1.384	1.383	1.387	1.386	1.379
C11-C12	1.393	1.393	1.394	1.394	1.394	1.396	1.4
C12-C13	1.405	1.407	1.405	1.406	1.409	1.406	1.408
C13-C14	1.534	1.535	1.536	1.543	1.538	1.54	1.547
C14-C15	1.555	1.557	1.552	1.554	1.557	1.556	1.558
C15-C16	1.535	1.537	1.542	1.538	1.536	1.546	1.535
C16-C17	1.517	1.521	1.52	1.521	1.519	1.511	1.519
C17-C18	1.539	1.546	1.545	1.535	1.543	1.536	1.541
C18-C19	1.504	1.503	1.505	1.508	1.503	1.499	1.504
C19-C2	1.413	1.414	1.417	1.413	1.411	1.416	1.414
C4-C17	1.528	1.524	1.533	1.525	1.527	1.54	1.522
C6-C15	1.507	1.51	1.509	1.505	1.514	1.509	1.516
C8-C13	1.419	1.419	1.423	1.424	1.417	1.421	1.43

Classical MD Simulation details: The analysis of MD simulations was carried out by using analytical tools which are implemented in GROMACS 5.0.7, such as gmx_mpi mindist, g_energy_mpi and g_rdf_mpi etc. As for the minimum distance, we created an index including GO and each individual TC molecule, and then, applied the “gmx_mpi mindist” to calculate the minimum distance between GO and TC molecule. While, the potential energy was calculated by using the tool of “g_energy_mpi”. The “LJ-SR” and“Coul-SR” interaction energies were chosen to calculate the potential energies between GO and three kinds of TCs molecules.