Supporting Information

Development of Fluorescent Carbon Nanoparticles from Madhuca Longifolia Flower for Sensitive and Selective Detection of Cr^{6+}: A Collective Experimental-Computational Approach

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(Fig. S1a)

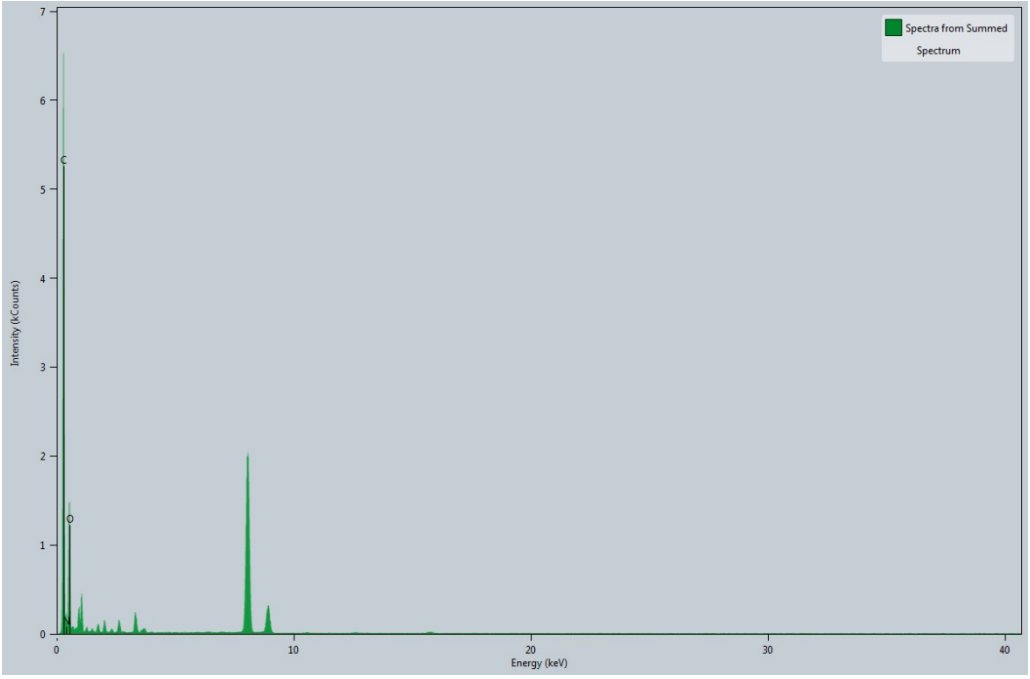

Fig. S1: EDS spectra of CNPs for determining elemental composition.

(Fig. S1b)

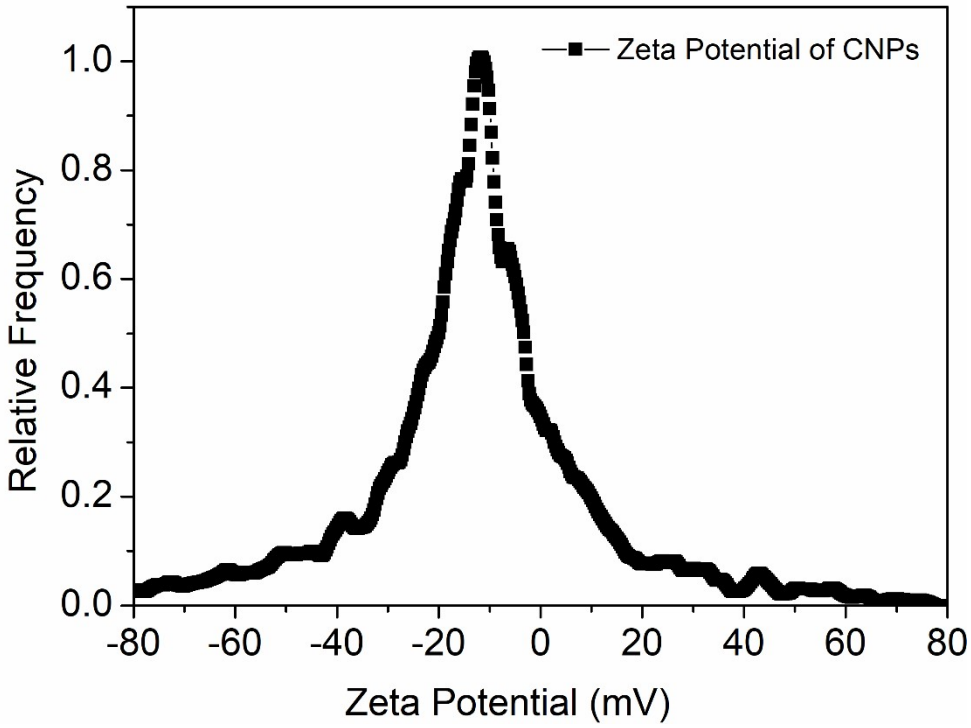

Fig. S1b: Zeta potential plot for the determination of the nature of functional groups and stability of water-dispersed CNPs

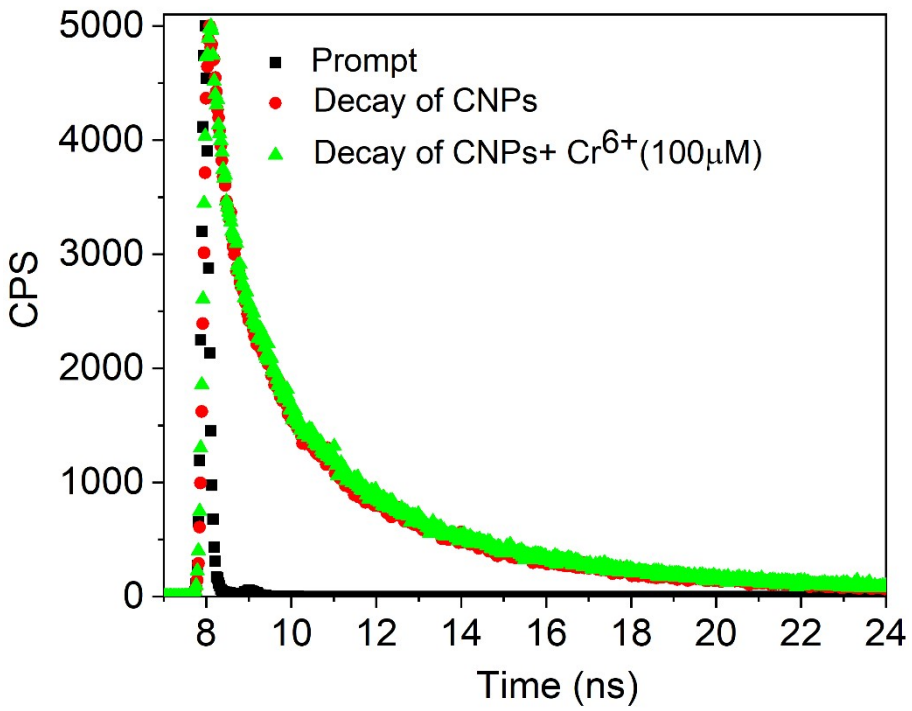

Fig. S2: Fluorescence life-time decay plot for CNPs (2.0 mg/mL) in the presence of 100 μM of Cr^{6+} (λ_{exc}= 405 nm and λ_{emi}= 490 nm).

Theoretical Study

For the sake of clarity, the QTAIM based molecular graphs of the free functionalized CNP constituent, Cr^{6+}@CNPc, and Cr^{6+}@CNPt have been shown in **Fig. S3**, **Fig. S4**, and **Fig. S5**, correspondingly.

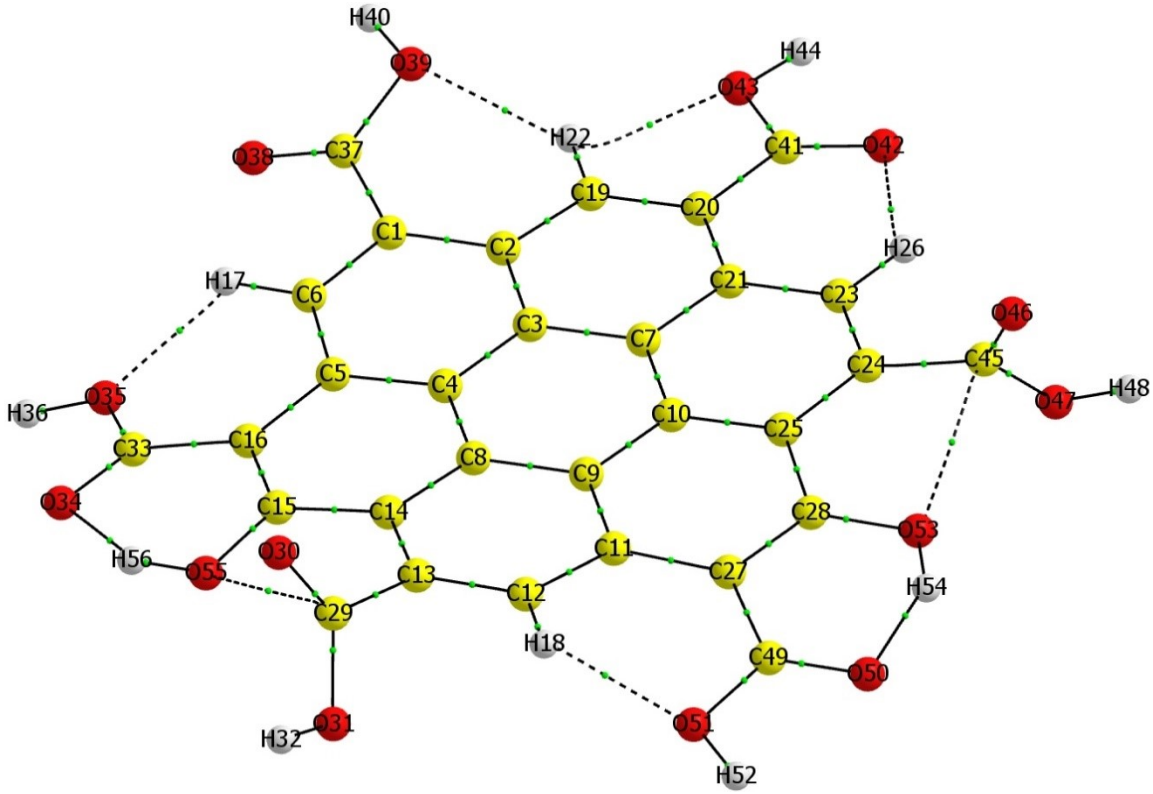

Fig. S3. The QTAIM Molecular Graph of the Free Functionalized CNP Moiety.

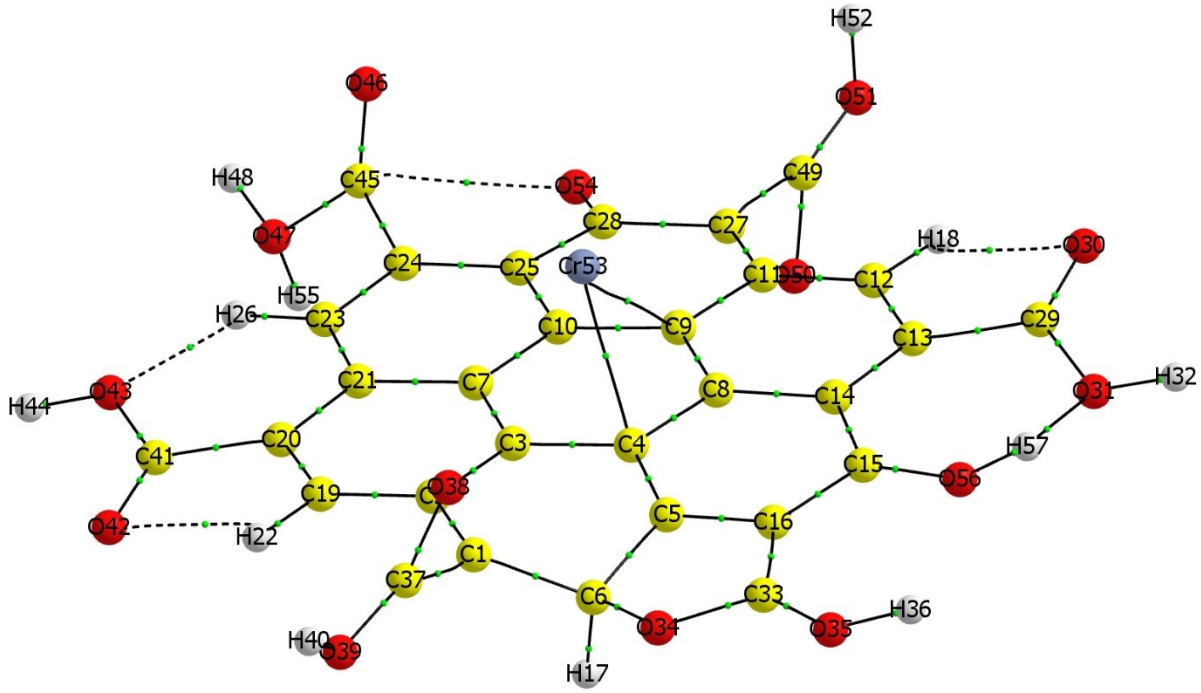

Fig. S4. The QTAIM Molecular Graph of the Cr^{6+} ion Interacting with the Functionalized CNP to form Complex Cr^{6+}@CNPc in the Centre of the CNP Moiety.

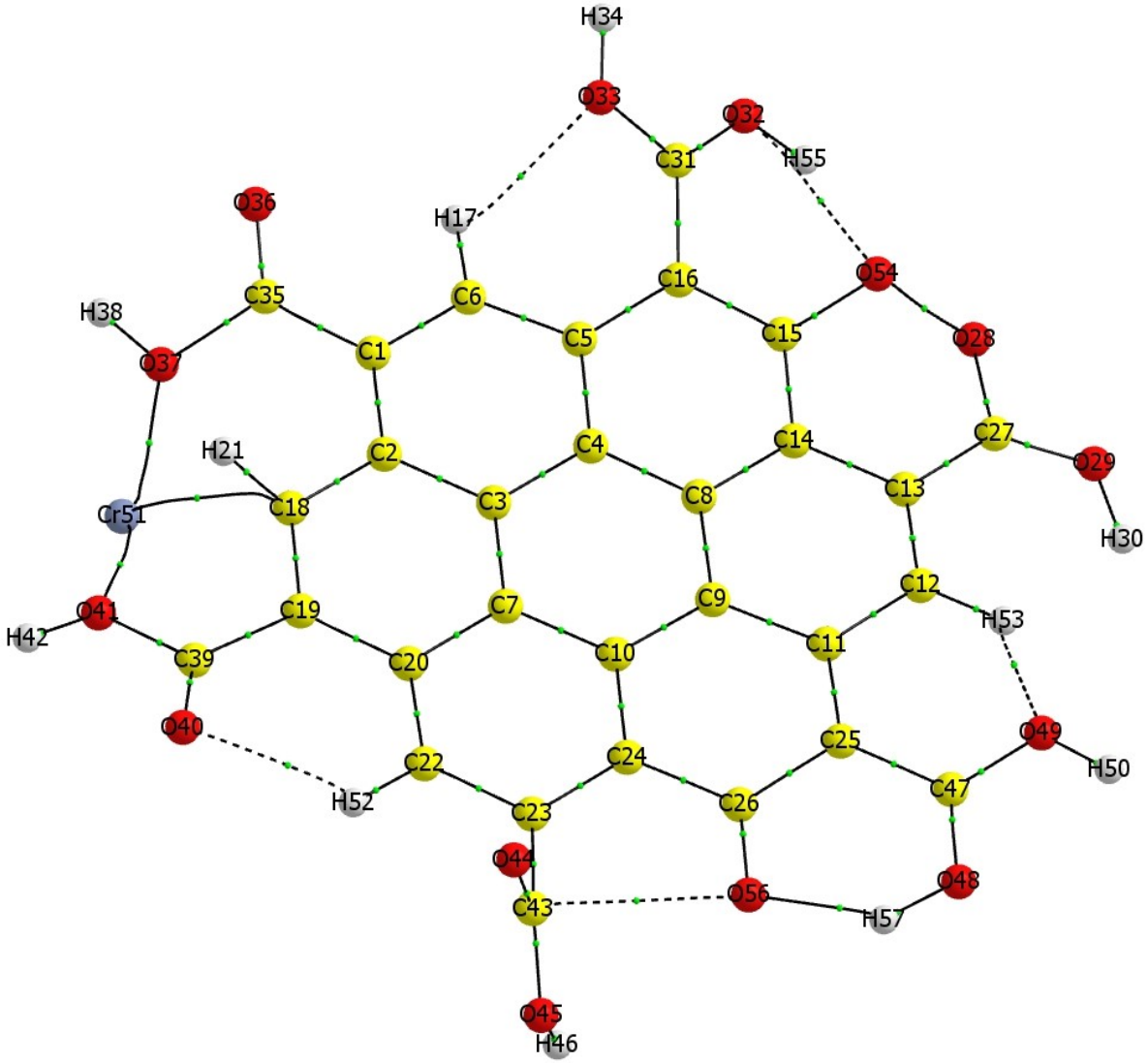

Fig. S5. The QTAIM Molecular Graph of the Cr^{6+} ion Interacting with the Functionalized CNP to form Complex Cr^{6+}@CNPt at the Terminal of the CNP Moiety.

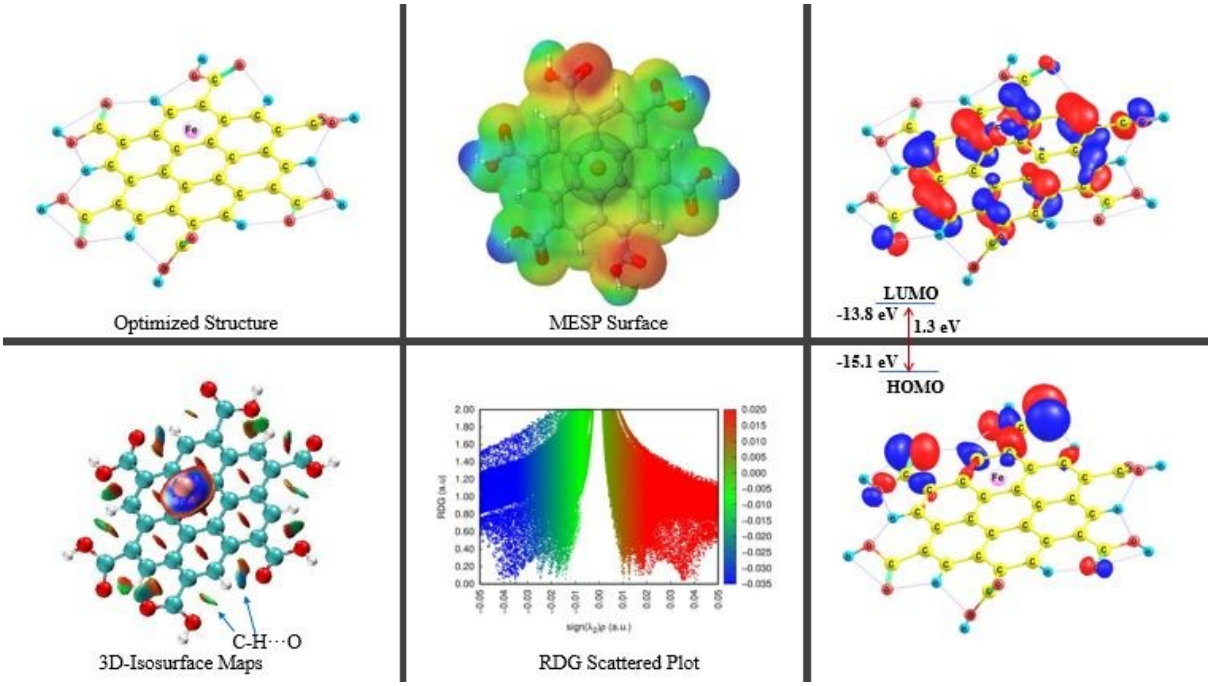

Fig. S6a. The Optimized Structure, MESP Surface, HOMO-LUMO 3D Maps, 3D-Isofurface Maps, and RDG Scattered Plot of the Fe^{3+} Interacting with the Functionalized CNP to form Complex Fe^{3+}@CNP in the Centre of the CNP Moiety.

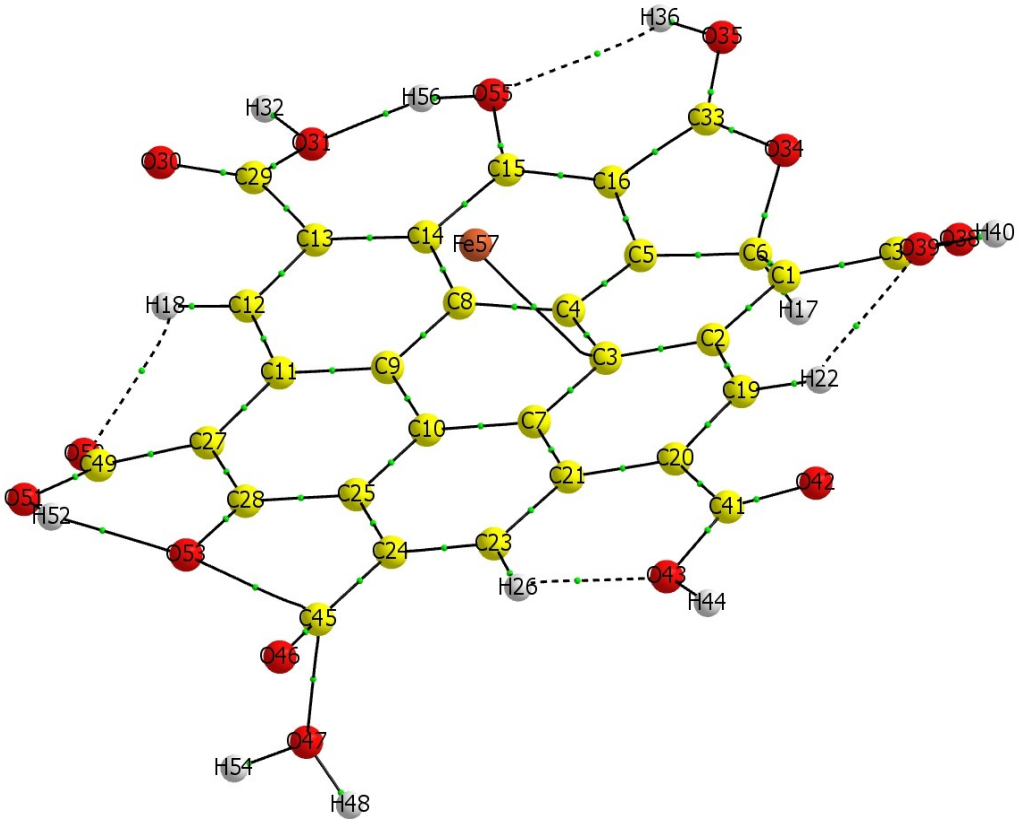

Fig. S6b. The QTAIM Molecular Graph of the Fe^{3+} ion Interacting with the Functionalized CNP to form Complex Fe^{3+}@CNPc in the Centre of the CNP Moiety.

Table S1. The QTAIM Data for the Fe^{3+} (in the Centre) Interacting with the Functionalized CNP Moiety.

Fe^{3+}@CNP (Centre)						
BP	**BL (Å)**	**BPL (Å)**	**ρ (au)**	**$\nabla^2(\rho)$ (au)**	**V (au)**	**DI (A, B)**
MNI						
C3─Fe57	2.336	2.392	0.0423	+0.1960	-0.0454	0.233
NCI						
O55-H56···O31	1.566	1.594	0.0616	+0.1961	-0.0573	0.132
O51-H52···O53	1.923	1.951	0.0287	+0.0962	-0.0248	0.063
C23-H26···O43	2.054	2.078	0.0226	+0.0840	-0.0185	0.065
C12-H18···O50	2.156	2.220	0.0198	+0.0765	-0.0153	0.052
C19-H22···O39	2.216	2.249	0.0167	+0.0613	-0.0129	0.047
O35-H36···O55	2.343	2.392	0.0107	+0.0419	-0.0088	0.022
	NBP					
C45···O47	2.240	2.242	0.040873	+0.103951	-0.029038	0.190157
C45···O53	2.364	2.373	0.030767	+0.085094	-0.020268	0.143337

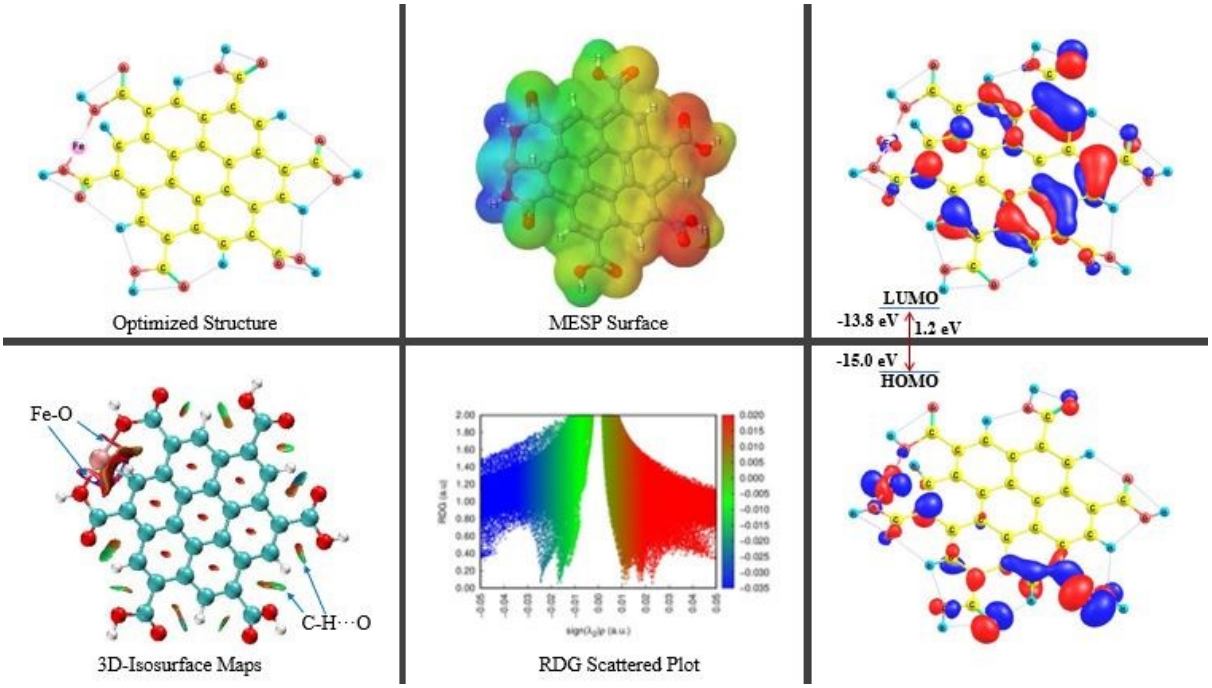

Fig. S7a. The Optimized Structure, MESP Surface, HOMO-LUMO 3D Maps, 3D-Isofurface Maps, and RDG Scattered Plot of the Fe^{3+} Interacting with the Functionalized CNP to form Complex, Fe^{3+}@CNPt at the Terminal of the CNP Moiety.

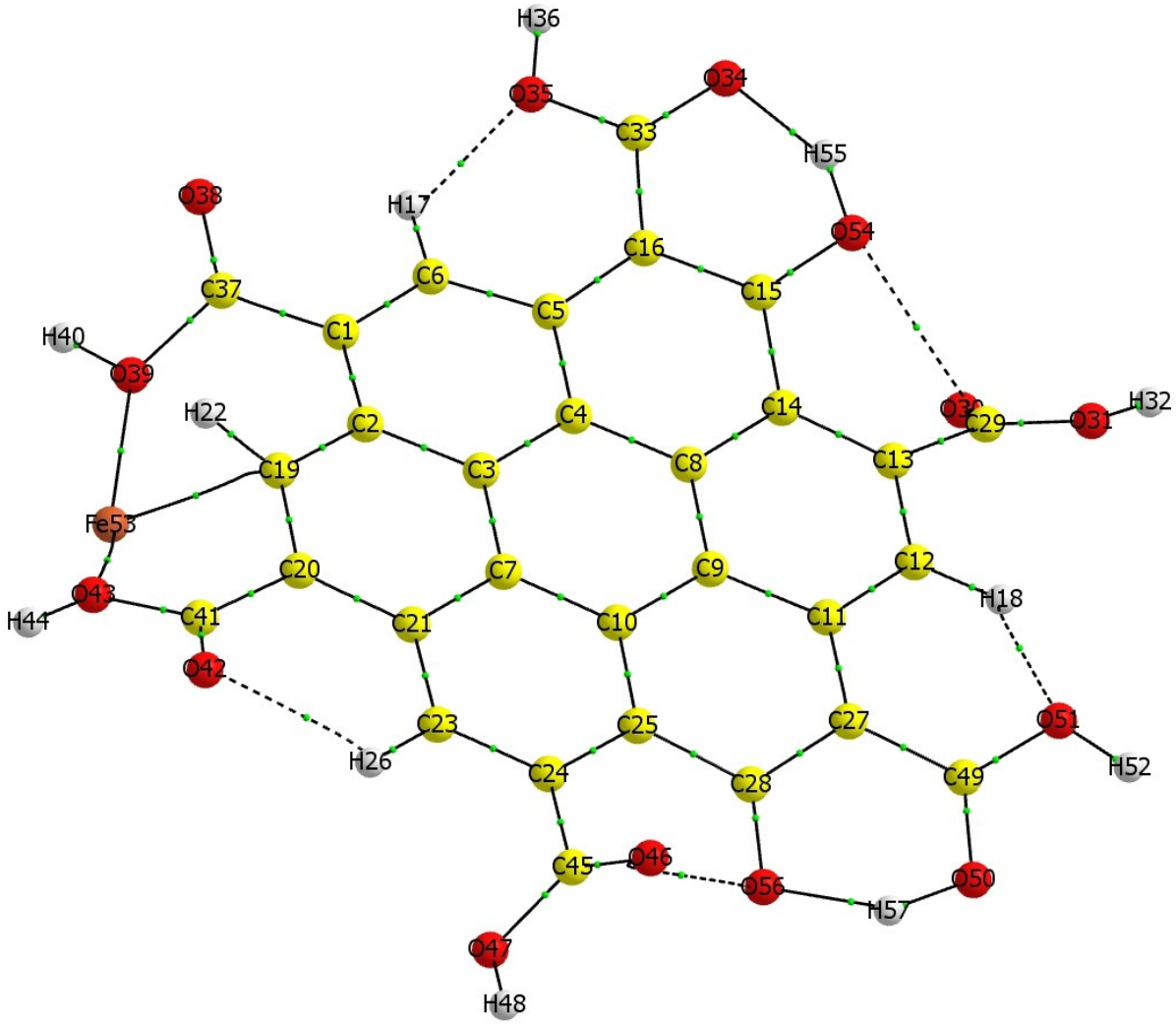

Fig. S7b. The QTAIM Molecular Graph of the Fe^{3+} ion Interacting with the Functionalized CNP to form Complex Fe^{3+}@CNPt at the Terminal of the CNP Moiety.

Table S2. The QTAIM Data for the Fe^{3+} (at the Terminal) Interacting with the Functionalized CNP Moiety.

Fe^{3+}@CNP (Terminal)						
Atoms	**BL (Å)**	**BPL (Å)**	**ρ (au)**	**$\nabla^2(\rho)$ (au)**	**V (au)**	**DI (A, B)**
MNI						
Fe53─O39	2.091	2.092	0.0545	+0.3990	-0.0892	0.368
Fe53─O43	2.089	2.101	0.0568	+0.3931	-0.0880	0.358
Fe53─C19	2.236	2.255	0.0537	+0.1918	-0.0558	0.336
NCI						
O50-H57···O56	1.467	1.485	0.0830	+0.1929	-0.0817	0.172
O54-H55···O34	1.503	1.524	0.0751	+0.2037	-0.0723	0.156
C6-H17···O35	2.040	2.065	0.0231	+0.0881	-0.0190	0.064
C12-H18···O51	2.137	2.167	0.0191	+0.0736	-0.0151	0.053
C23-H26···O42	2.220	2.260	0.0164	+0.0614	-0.0123	0.049
NBP						
O56···O46	2.745	3.077	0.0151	+0.0595	-0.0113	0.072
O30···O54	2.767	3.283	0.0150	+0.0611	-0.0115	0.064

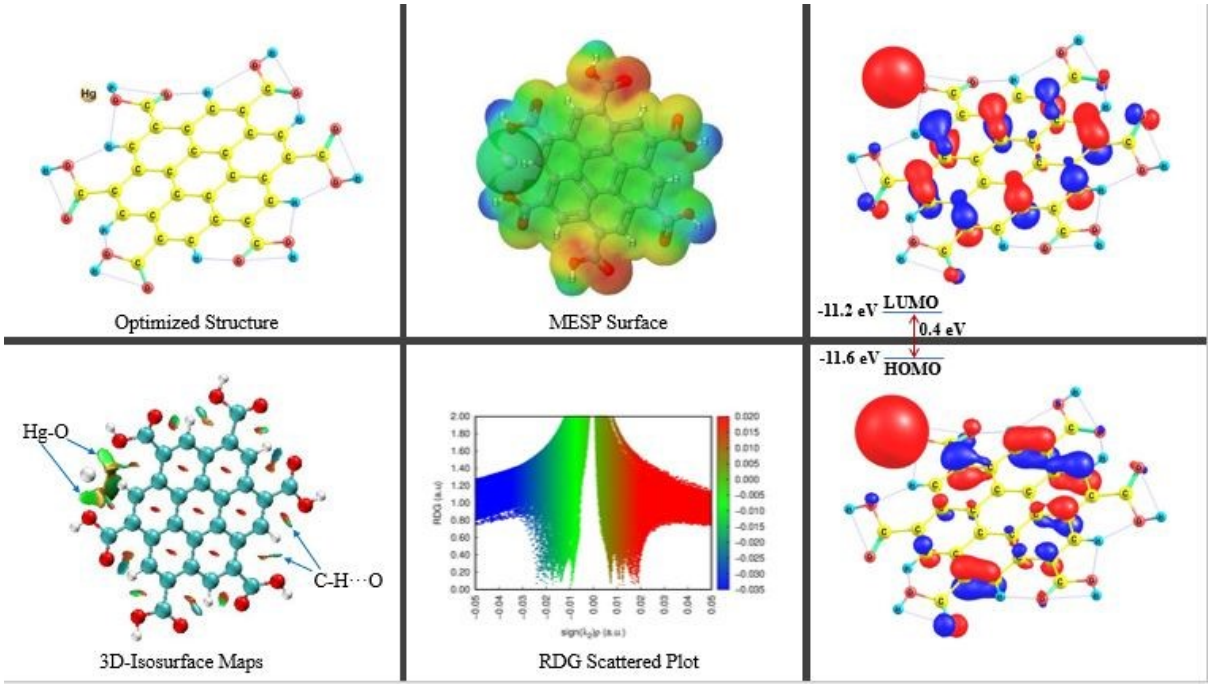

Fig. S8a. The Optimized Structure, MESP Surface, HOMO-LUMO 3D Maps, 3D-Isofurface Maps, and RDG Scattered Plot of the Hg^{2+} Interacting with the Functionalized CNP to form Complex Hg^{2+}@CNPt at the Terminal of the CNP Moiety.

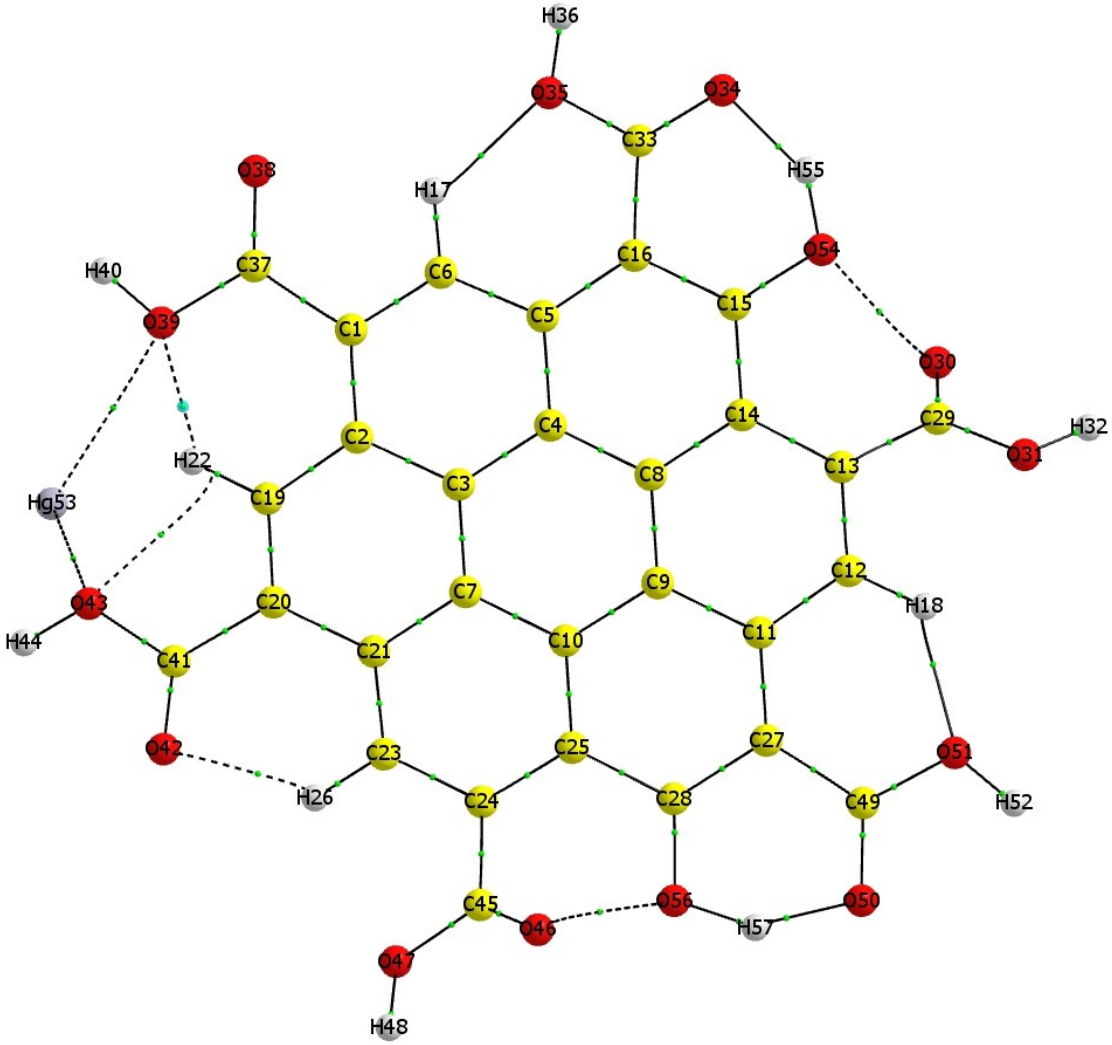

Fig. S8b. The QTAIM Molecular Graph of the Hg^{2+} ion Interacting with the Functionalized CNP to form Complex.

Table S3. The QTAIM Data for Hg^{2+} (at the Terminal) Interacting with the Functionalized CNP Moiety.

Hg^{2+}@CNP (Terminal)						
Atoms	**BL (Å)**	**BPL (Å)**	**ρ (au)**	**$\nabla^2(\rho)$ (au)**	**V (au)**	**DI (A, B)**
MNI						
Hg53─O39	3.153	3.157	0.0108	+0.0305	-0.0067	0.097
Hg53─O43	2.943	2.944	0.0163	+0.0491	-0.0116	0.143
NCI						
O56-H57···O50	1.415	1.429	0.0944	+0.1732	-0.0990	0.197
O54-H55···O34	1.522	1.542	0.0715	+0.2050	-0.0683	0.150
C6-H17···O35	1.961	1.984	0.0272	+0.1051	-0.0232	0.073
C12-H18···O51	1.988	2.010	0.0258	+0.0992	-0.0217	0.072
C19-H22···O39	2.019	2.040	0.0246	+0.0917	-0.0207	0.070
C23-H26···O42	2.057	2.083	0.0236	+0.0841	-0.0191	0.069
C19-H22···O43	2.259	2.601	0.0173	+0.0830	-0.0140	0.036
NBP						
O46···O56	2.632	2.658	0.0175	+0.0688	-0.0138	0.082
O30···O54	2.636	2.655	0.0174	+0.0681	-0.0138	0.080