

List of Figures

Figure 1.1	Road map of carbon materials - from graphite to graphene quantum dots.	2
Figure 1.2	Preparation methods of graphene quantum dots.	5
Figure 1.3	Schematic of the functionalization of GQDs through different routes and enhancement of its properties. Reproduced from Tian et al. Mater. Today Chem. 10, 221 (2018). Copyright 2018 Author(s), licensed under the Creative Commons License.	8
Figure 1.4	Applications of GQDs in different fields. Reproduced from Tian et al. Mater. Today Chem. 10, 221 (2018). Copyright 2018 Author(s), licensed under the Creative Commons License.	10
Figure 2.1	Demonstration of Kohn-Sham ansatz. The HK_0 represents Hohenberg and Kohn theorem for non-interacting system. The link between many body and the independent particle system is provided by Kohn – Sham (KS).	29
Figure 2.2	The PES curve presenting minima, transition states, saddle points along with reaction paths. Reproduced with permission from Keil, Comput. Math. Appl. 65, 1674 (2013). Copyright 2013 Elsevier.	37
Figure 3.1	Ground state geometries of triangulene with (a) Antiferromagnetic (AFM) (b) Ferromagnetic (FM) structure with atomic numbering scheme. The carbon and hydrogen atoms respectively are determined by the blue and red spheres.	45
Figure 3.2	Optimized geometries of triangulene with (a) Iron (b) Cobalt (c) Nickel and (d) Copper adatoms along with top and side view. The green, fluorescent, orange, and light blue balls represent iron, cobalt, nickel and copper atoms respectively.	46
Figure 3.3	Raman spectra of both (a) AFM (b) FM phases of triangulene.	49
Figure 3.4	Several Raman and IR molecular vibrations of triangulene. (a-c) presents the out-of-plane vibrations and (d-e) presents in-plane vibrations.	49
Figure 3.5	Electronic DOS for (a) AFM, alpha-FM and beta-FM phases of triangulene, and (b) transition metal elements adsorbed triangulene.	51
Figure 3.6	HOMO and LUMO levels of triangulene (a) AFM (b) alpha-FM (c) beta-FM.	52
Figure 3.7	HOMO and LUMO levels of triangulene (a) Fe (b) Co (c) Ni (d) Cu.	53
Figure 3.8	MESP plotted for (a) AFM triangulene ranging -2.102×10^{-2} (red) to $+2.102 \times 10^{-2}$ (blue). (b) FM triangulene ranging -2.043×10^{-2} (red) to $+2.043 \times 10^{-2}$ (blue).	54

Figure 4.1	(a) Initial and (b) optimized geometries of hydrogen atom over triangulene along with top and side views.	62
Figure 4.2	(a) Side view of initial geometry of hydrogen over triangulene positioned at the edge and (b) optimized structure of hydrogen over edge of GQD depicting covalent interaction.	63
Figure 4.3	DOS of pristine triangulene and hydrogen over triangulene. The vertical freckled line presents the HOMO level energy.	64
Figure 4.4	Initial geometries of Pt on triangulene with (a) bridge (b) hollow and (c) top sites.	65
Figure 4.5	Optimized geometries of Pt adsorbed triangulene for sites (a) bridge (b) hollow and (c) top.	66
Figure 4.6	Initial geometries of H ₂ on Pt adsorbed triangulene with different sites (a) bridge (b) hollow and (c) top.	67
Figure 4.7	Optimized geometries of H ₂ on Pt adsorbed triangulene for all three sites (a) bridge (b) hollow and (c) top.	68
Figure 4.8	DOS of (a) Pt over triangulene (b) H ₂ on tri+Pt for all considered sites.	69
Figure 4.9	HOMO-LUMO surfaces of H ₂ over tri+Pt with (a) bridge, (b) hollow and (c) top sites.	70
Figure 5.1	Illustration of photoinduced electron injection from a donor GQD to the surface of acceptor TiO ₂ . The photon absorption benefits an electron from the GQD ground state with energy within E _g of TiO ₂ , into the excited state.	78
Figure 5.2	Optimized configuration of (a) carboxyl functionalized GQD (b) nitrogen doped COOH-GQD (c) boron doped COOH-GQD and (d) phosphorus doped COOH-GQD.	79
Figure 5.3	HOMO-LUMO curve for all considered systems of COOH-GQDs.	82
Figure 5.4	MESP surfaces for (a) carboxyl functionalized GQD (b) nitrogen doped COOH-GQD (c) boron doped COOH-GQD and (d) phosphorus doped COOH-GQD.	83
Figure 5.5	Mulliken graph for all considered systems.	85
Figure 5.6	UV-Vis curve of all considered systems.	87
Figure 5.7	Tauc plot of all considered systems.	88
Figure 5.8	Evaluated J-V curve at temperature T=300K.	90
Figure 6.1	Optimized geometries of GQDs with (a) oxygen doped GQD and (b) sulphur doped GQD.	99
Figure 6.2	Initial geometries of (a) Mel-O-GQD and (b) Mel-S-GQD.	100
Figure 6.3	HOMO-LUMO surfaces of (a) Mel-O-GQD and (b) Mel-S-GQD.	101
Figure 6.4	MESP surfaces of (a) pristine melamine (b) O-GQD (c) S-GQD (d) Mel-O-GQD and (e) Mel-S-GQD.	102

Figure 6.5	MPA of (a) pristine melamine (b) O-GQD (c) S-GQD (d) Mel-O-GQD and (e) Mel-S-GQD.	103
Figure 6.6	Theoretical Raman spectra of melamine, Mel-O-GQD and Mel-S-GQD ranging between (a) 200 cm^{-1} to 800 cm^{-1} and (b) 1000 cm^{-1} to 1600 cm^{-1} .	104
Figure 6.7	Initial and optimized geometries of (a) hollow melamine-GQD (b) top melamine-GQD and (c) bridge melamine-GQD.	107
Figure 6.8	((a) Top view and (b) side view of optimized geometries of melamine over f-GQDs.	108
Figure 6.9	HOMO-LUMO levels of melamine and melamine over f-GQD.	109
Figure 6.10	Plot of Raman spectra of (a) pristine melamine and (b) SERS of f-GQD-mel.	110
Figure 7.1	Magnetic moment of pristine and iron, cobalt, nickel, copper doped triangulene depicting their superiority.	116
Figure 7.2	Schematic of adsorption energy trend of H_2 over Pt decorated triangulene	117
Figure 7.3	Schematic of photo-induced injection of electrons from COOH-GQD into the surface of TiO_2 .	118
Figure 7.4	Schematic of melamine adsorbed on O-GQD and f-GQD along with their SERS.	119
Figure 7.5	Challenges for GQDs that are needed to be addressed.	120