List of Tables

Table 3.1	The ground state energy and calculated dipole moment for pristine and doped triangulene.	47
Table 3.2	Calculated energies of HOMO-LUMO, HOMO-LUMO gap (E_g) , adsorption energy (E_{ad}) and magnetic moment (M) of all considered systems.	48
Table 3.3	Raman and IR vibrational assignments for FM and AFM phases of triangulene.	50
Table 3.4	Calculated HOMO and LUMO energies (eV) along with global reactivity parameters.	53
Table 4.1	Computed HOMO, LUMO, HOMO-LUMO gap (E_g) and adsorption (E_{ad}) energies of triangulene and hydrogen over triangulene.	63
Table 4.2	Calculated HOMO, LUMO, E_g and E_{ad} energies of all considered systems	66
Table 5.1	Computed HOMO (E_{HOMO}), LUMO (E_{LUMO}) energies, HOMO-LUMO gap (E_{g}), electron affinity (EA) and work function (WF) of all considered systems.	81
Table 5.2	Evaluated maximum absorption wavelength, λ_{max} (nm), electronic transition energy (eV), oscillator strength (f) and light harvesting energy (LHE) of all systems.	86
Table 5.3	Computed solar cell parameters of systems.	90
Table 6.1	Computed HOMO and LUMO energies, HOMO-LUMO gap (E_g) and adsorption energy (E_{ad}) of all systems.	101
Table 6.2	Calculated Raman spectral data and vibrational assignments of pristine melamine, Mel-O-GQD and Mel-S-GQD.	105
Table 6.3	Evaluated enhancement factor (EF) of Mel-O-GQD and Mel-S-GQD.	106
Table 6.4	Calculated adsorption energy (E_{ad}) of melamine on GQD and f -GQD for all three sites.	108
Table 6.5	Evaluated Raman wavenumbers of melamine and <i>f</i> -GQD-mel in cm ⁻¹ together with EF.	111