List of Tables

3.1	The theoretical values of E_{VB} eV, and E_{CB} eV for all the metal-non
	metal functionalized CN
3.2	The theoretical values of E_F , E_{vac} , Φ , E_{BGC} , and β for CN , B_{int} -
	CN , $B_{non-int}$ - CN , Co - CN , $(Co$ - $B)_{int}$ - CN , and $(Co$ - $B)_{non-int}$ - CN 58
5.1	The calculated for cohesive energy (E_{coh}) , interlayer distance dif-
	ference (ΔD) , band gap (E_q) , Fermi energy (E_F) , vacuum energy
	(E_{vac}) , work function (Φ) , band gap center (E_{BGC}) , effective mass
	of holes $(m_h^*(m_0))$, electrons $(m_e^*(m_0))$, effective mass ratio (β) and
	integrated absorption (α)
5.2	Charge difference for BL - CN [9] and Li - CN between the upper &
	and lower layers
5.3	The ΔQ_{il} interlayer charge difference and the adsorption energy for
	the reaction intermediates of OER and HER for the Li - CN system. 122