List of Figures

1.1	The steps involved in the photocatalysis mechanism with possible ways of charge carrier recombination.	3
1.2	Various band edge positions across the reduction-oxidation potential for feasible/prohibitive reaction, potential scale is shown against	
	E_{vac}/NHE	4
1.3 1.4	Different functionalization techniques shown in the sequential form. (a) Band Edges for experimental and theoretical pristine and non-	7
	metal doped g- C_3N_4 [1], (b) Band Edges for metal and anion-cation doped g- C_3N_4 (Potential vs E_{vac})	10
1.5	Different types of heterostructure, Schottky junction within metal- semiconductor interface, type-II and z-scheme categorized for	
	semiconductor-semiconductor heterojunction	13
2.1	Picture of an elephant surrounded by numerous bees representing the sluggish-nuclei, and electrons orbiting, respectively around it	27
2.2	Flow diagram (Self-consistent field cycle) showing the steps involved in computing a solid's total energy using traditional matrix diago-	
2.3	nalization	32
2.0	all-electron (solid lines) and pseudoelectron (dashed lines) potentials. The suggested radius (r_c) is the one at which the values of all	0.0
2.4	electrons and pseudoelectrons match. [2]	36 37
2.5	According to the Lorentz oscillator model, the real component ϵ_1 and the imaginary part ϵ_2 of the dielectric function path are shown	
2.6	in the picture as being dependent on the frequency ω [3] Climbing Image Nudge Elastic Band plot showing the minimum energy path, along with the tangential forces to compute the reaction	42
	barrier [4, 5]	45
2.7	E-k diagram representing bands of different curvature, and the parabolic fitting specifying the curvature depending on mobility	46
3.1	Pristine structure with N^{edge} , N^{tri} . N^{bridge} , C^{cor} , N^{bay} , triazinemesh, void, and pore for CN tri-s-triazine form	54

Optimized structure of (a) pristine CN , (b) B_{int} - CN , (c) $B_{non-int}$ - CN , (d) Co , CN , (e) $(Co - R)$, CN , and (f) $(Co - R)$, CN	58
	90
	59
· · · · · · · · · · · · · · · · · · ·	00
() []	
(" /[]/ 0	
	62
$(Co-B)_{non-int}$ - CN	65
The Gibbs free energy plot for HER over Pt, CN , B_{int} - CN ,	
$B_{non-int}$ - CN , Co - CN , $(Co - B)_{int}$ - CN , and $(Co - B)_{non-int}$ - CN ,	
using H/H_3O adsorbate	67
(a. a. a) Initial and (b. d. f) antimized attracture for (CaP)0D CN	
	75
	10
	77
CN , and (i-1) $(CoB)_2^{2D}$ - CN	78
(a, b, c) Planar averaged charge density difference and, (d, e, f)	
electrostatic potential profile for $(CoB)_2^{0D}$ - CN , $(CoB)_4^{0D}$ - CN , and	
$(CoB)_2^{2D}$ - CN , yellow and cyan represent charge accumulation and	
depletion, inset shows magnified version in small range	79
	0.0
	80
	81
	88
	00
	89
	90
	30
	91
	CN , (d) Co - CN , (e) $(Co - B)_{int}$ - CN , and (f) $(Co - B)_{non-int}$ - CN . The PDOS for (a) pristine CN , (b) B_{int} - CN , (c) $B_{non-int}$ - CN , (d) Co - CN , (e) $(Co - B)_{int}$ - CN , and (f) $(Co - B)_{non-int}$ - CN . Zero energy is used to signify E_F . The corresponding atom's s-orbital is shown by the shaded region. (a) E_{VB} and E_{CB} experimental values for bulk (@)[6] and nanosheet(#)[7], together with band edges plot using various functional (PBE-GGA and HSE06), (b) Absorbance coefficient, and (c) imaginary part of dielectric function for CN , B_{int} - CN , $B_{non-int}$ - CN , Co - CN , $(Co - B)_{int}$ - CN , and $(Co - B)_{non-int}$ - CN . The Gibbs free energy plot for OER over (a) pristine CN , (b) B_{int} - CN , (c) $B_{non-int}$ - CN , (d) Co - CN , (e) $(Co - B)_{int}$ - CN , and (f) $(Co - B)_{non-int}$ - CN . The Gibbs free energy plot for HER over Pt, CN , B_{int} - CN , $B_{non-int}$ - CN , $B_{non-int}$ - CN , and $B_{non-int}$ - $B_{$

. 93	(a) Electrostatic potential profile, (b) Plane-averaged charge density difference of heterostructure along z-direction normal to the heterostructure. The 3D isosurface is the charge density difference where magenta and cyan areas represent electron accumulation and depletion, respectively, (c) Absorption coefficient: inset(imaginary part of dielectric function), and (d) band edges position of pristine and heterostructure.	4.11
. 94	Gibbs free energy profile for (a) CN , (b) Hf_2CO_2 , intermediate adsorbed over Hf_2CO_2/CN over (c) lower, and (d) upper surface for oxygen evolution reaction and (e) H-atom, (f) H_3O , intermediate for hydrogen evolution reaction.	4.12
. 100	Initial and optimized structure in top and side configuration has been demonstrated for $S_0 - S_8$ bilayer arrangement of CN	5.1
n. 105 . 106	Illustration of total, partial DOS for $S_0 - S_8$ bilayer- CN configuratio Orbital DOS for S_0 , corrugated- S_3 , and planar- S_5 bilayer geometry for CN .	5.2 5.3
	(a, c, e) Highest occupied molecular orbital (HOMO), (b, d, f) Lowest unoccupied molecular orbital (LUMO) top and side view and (g, h, i) 2D ELF contour (1 0 0 slab) for ML, S_3 and S_5 , respectively	5.4
. 107	(a) Band edges for ML, S_0 - S_8 CN configuration, (b) absorbance, and (c) imaginary part of dielectric function for ML, S_5 , S_3 geometry for HSE functional. Inset represents $\alpha(\omega)$ and $\epsilon_2(\omega)$ for PBE	5.5
	(a, b) Sites over the upper/lower face of S_3 , (c-h) Gibbs free energy for OER, (i, j) for HER over respective sites. HER includes ML and Pt for reference.	5.6
. 126	Band dispersion curve for Li - CN using Wannier functions that are	5.7
	A side view of the Li - CN crystal structure shows the (a) basic and (b) optimized structures; (c) the total, sum of the partial density of states for all atoms in the upper and lower layers of the material,	5.8
	along with bands and the Fermi energy shifted to zero With Fermi energy shifted to zero, the local and partial density of states for Li - CN and atoms involved in interlayer contact via Li	5.9
	bridging. (a) The electrostatic potential profile illustrates the potential variance with cell length (z-axis). The inset shows how the peak locations of LL and UL vary. Isosurface shows the perspective for (b) BL - CN , and (c) Li - CN electron localization functions for Li - CN . (d) For Li - CN , the absorption coefficient (α) & imaginary component of the dielectric function versus energy is shown, with the energy range between 2.6 and 3.8 eV highlighted in the inset, and (e) BL - CN , Li - CN , and CN ML's Reduction-Oxidation potential against the NHE/ E_{vac} *[8]	5.10

5.11	(a) An enhanced configuration (unit cell) with designated sites for intermediate adsorption; (b) A Gibbs free energy profile for the process of the oxygen evolution reaction, encompassing Sites 1-6	
	throughout Li - CN	. 132
5.12	Profile of Gibbs free energy for the evolution of hydrogen, encompassing Sites 1-6 over Li - CN	. 133
5.13	Sequential oxygen evolution reaction & hydrogen evolution reaction over Li - CN in a cyclic process	. 133
5.14	(a-e) Electrostatic potential plot and, (f-j) ELF for simultaneous OER and HER	. 134
5.15	The Li - CN surface is used to accomplish the free energy change for OER and the activation barrier for OER+HER	. 137
5.16	(a-d) Charge density difference isosurface plot for pristine plotted at different orientations, blue and yellow region indicate charge lost	190
5.17	and gained, respectively	. 138
5.18	CN using $\Delta \rho_1 = \rho_{system} - (\rho_{2H_2O} + \rho_{Li-CN})$. 130
5.19	$ \rho_{LiCN_{UL}} $)	
	$ ho_{LiCN_{UL}})$. 138
6.1	Possible reaction intermediates for CO_2RR over $Co-CN$	
6.2 6.3	Possible reaction intermediates for N_2RR over $Co-CN$ Reaction pathways followed of CO_2RR including the possible reaction of CO_2RR including the possible reaction.	
6.4	tion intermediates for $Co - CN$	
6.5	(a) Optimized structure, (b) Charge density difference, and (c) electron localization function plotted for $Co - CN$.	
6.6	Distinct reaction pathways for CO_2RR over $Co-CN$	
6.7	Most feasible reaction pathway with lowest energy barrier for CO_2RR over $Co-CN$	
6.8	Distinct reaction pathways for N_2RR over $Co-CN$. 157
6.9	Most feasible reaction pathway with lowest energy barrier for N_2RR over $N-CN$. 158
7.1	Overpotential, and band edges schematics for different functionalization over CN -photocatalyst	. 162