7 | Conclusions and Future Prospects

In the context of the rationale and goals described in chapter 1 of this thesis, this chapter summarizes the findings and conversations from earlier chapters. In this chapter, we highlight and reiterate the remarkable outcomes of our first-principles research while briefly mentioning the thesis' salient elements. We also touch on the future potential covered in this thesis, as well as possibilities to explore $g-C_3N_4$ based photocatalysts.

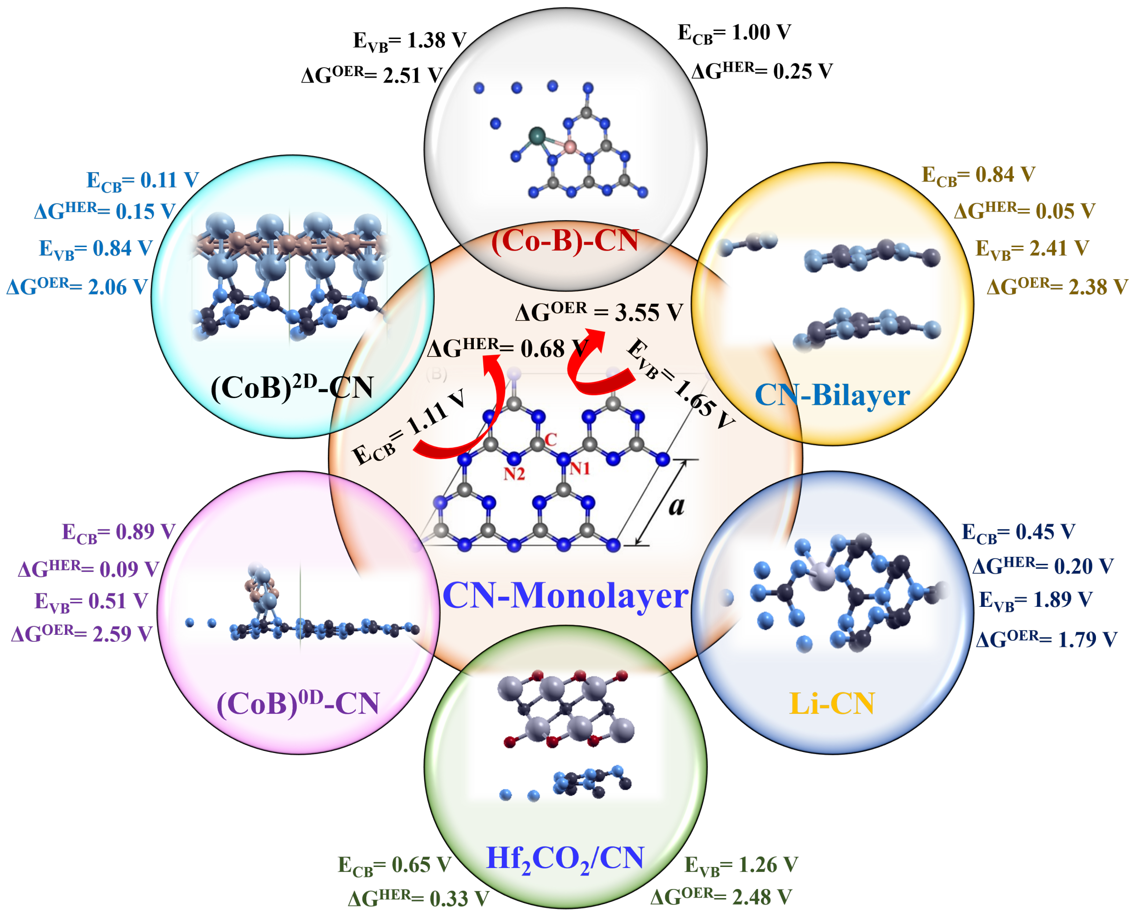

FIGURE 7.1: Overpotential, and band edges schematics for different functionalization over CN-photocatalyst.

7.1 Conclusions

As a conclusion of all the chapters (1-3), various functionalization techniques have been utilized and discussed to understand its dependence on the reaction overpotential. With the initialization of Cation-loading, anion-doping over CN, we see a narrowing of the band gap along with a reduction in the $\eta^{HER/OER}$ verifying its role on the increase of absorbance, and feasibility of reaction as seen from Fig. 7.1. Moving anti-clockwise next comes the design of CoB decorated CN in two configurations, $(CoB)^{oD} - CN$, and $(CoB)^{2D} - CN$ to utilize the synergistic effect of Co and B atoms in cluster and slab form, respectively. High performance in photocatalytic activity has been evidenced from $\eta^{HER/OER}$, along with red shifting of absorbance curve, and formation of a unidirectional charge transfer channel. This study has been further explored over the semiconductor-semiconductor heterojunction, where Hf-based MXene has been supported over CN. Hf_2CO_2/CN shows an alternating charge transfer pathway for spatial separation of photogenerated charge carriers for the reduction in the recombination rate, followed by reduced $\eta^{HER/OER}$ value in comparison to CN. The modification method used to corrugate the bilayer through orbital interaction and intercalation of alkali metal for interlayer charge transfer channel creation has shown extraordinary results with increment in the band gap value for bilayer accommodating the $\eta^{HER/OER}$ within band edges. Whereas, $Li-CN$ has further improved the overall water splitting efficiency by the lowest value of η^{OER} among the studied photocatalyst, $\eta^{HER/OER}$ smaller than band edges and optical absorption in the visible region of the spectrum making it perfect photocatalyst for complete water dissociation. The study then explores more about the reaction mechanism over the best-reducing photocatalyst among the studied for CO_2RR, and N_2RR.

7.2 Future Scope

The systematic study performed on the functionalization of the CN, its role in charge migration, separation, and recombination, along with its effect on the reaction barrier has helped to gain a deeper insight into various aspects. These include the various functionalization methods, computational tools to explore the properties of the material at an electronic level, reaction mechanisms, and the role of intermediates over surface physics. The need for conversion techniques of energy and the demand for energy production at a large scale directs us to propose the following as future work:

1. Computation of energy barrier using Gibbs free energy and activation barrier using CI-NEB for CO_2RR and N_2RR over TM-based single atom catalyst needs to be carried out.

2. A standard model to calculate the efficiency of photocatalysts based on their absorbance, Gibbs free energy, charge recombination, and losses during the

reaction needs to be formalized and considered for comparison of photocatalysts.

3. Excitonic dynamics in-situ reaction mechanism should be explored for increasing the efficiency of the photocatalyst as it governs the charge separation and the generation of photoinduced charge carriers.

4. Simulation of CO_2, N_2, and H_2 over the surface of photocatalyst for Urea oxidation reaction need to be explored in finer detail.

5. CO_2RR over the Martian surface needs to be simulated considering the geologically abundant material as a catalyst for CH_3OH production.