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Amine Functionalized Mo doped graphitic Carbon Nitride (g-C_3N_4) as efficient catalysts for CO2 Hydrogenation in plasma reactor

Aim

The efficient, cost-effective, and selective conversion of CO_2 into synthetic fuels and chemical precursors remains a significant 21st-century challenge. Efforts have explored catalytic pathways such as CO_2 hydrogenation, direct decomposition, and methane dry reforming. Among these, the reverse water gas shift (RWGS) reaction, converting CO_2 and H2 into CO, has garnered attention. However, its endothermic nature makes it energy-intensive, favouring high temperatures. Non-thermal plasma (NTP) offers a breakthrough by enabling CO_2 conversion under mild conditions, reducing costs. This study investigates Mo-doped graphitic carbon nitride (-NH_2 functionalized) as a catalyst in plasma reactors. The effect of Mo loading and amine functionalization will be studied and aim would be higher selectivity towards C1 products.

Justification

Energetic electrons produced in the NTP interact with reactants and carrier gases, producing a range of reactive species such as ions, radicals, and excited species. Coupling NTP with heterogeneous catalysis, known as plasma catalysis, has great potential to generate a synergistic effect due to the physicochemical interaction between plasma and catalysis, resulting in the enhanced conversion, selectivity and energy efficiency under mild reaction conditions. g-C_3N_4 (GCN), a two dimensional non-metallic carbonitride with tri-s-triazine (C6N7) units showed excellent catalytic activity for CO_2 as it possesses a unique exposed surface-rich Lewis base (-NH/NH_2) that acts as a nucleophilic site for CO_2 activation. Due to its highly electron-rich structures and the capability to donate electrons, GCN can act as a potential catalyst for activating CO_2 molecules. However, GCN typically has a bulky structure that limits its surface area and reactive sites. This can be addressed with proper exfoliation and intercalation with atoms. Mo doped GCN can enhance CO_2 hydrogenation reaction as homogeneous dispersion of Mo atoms simultaneously delaminates and fragments the GCN sheets. These atomically dispersed Mo (Lewis acid) and N-rich GCN nanosheets (Lewis base) can maximize the utilization of reaction sites for CO_2 activation along with plasma under mild reaction conditions.

Program

Methodology of the proposed work aims at Followings;

- Synthesis of pure phase Mo doped -NH2-g-C_3N_4 nanostructures by wet chemical route.
- The composition of prepared catalyst will be varied for different Mo loadings and the prepared nanostructures will be characterized (XRD, SEM, XPS, CO_2-TPD, H_2-TPR, BET adsorption-desorption).
- Testing in plasma reactor for varying concentration of feed gas.
- Kinetics, thermodynamic, selectivity & conversion with respect to variable parameters.