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EXPERIMENTAL AND THEORETICAL INVESTIGATION ON PHOTOCATALYTIC HYDROGEN PRODUCTION FROM WATER/METHANOL SOLUTIONS BY CUPROUS OXIDE AND CUPRIC OXIDE COMPOSITE CATALYST

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Water can be split into hydrogen and oxygen by using semiconductor metal oxide photocatalysts and solar energy. This is a clean and inexhaustible energy source, as both water and sunlight are plentiful. The goal of the present investigation was to generate hydrogen by photo-splitting water using a cuprous oxide-based nano photocatalyst. Using the hydrothermal methodology, a series of Cu_2O/CuO photocatalysts were produced by altering the processing conditions. The efficiency of the photocatalytic activity of the synthesized catalyst was studied using methanol/water (40/60%) mixtures. It was observed that the photocatalytic activity initially increased with increasing Cu_2O content in the catalyst and then decreased. According to XRD characterization of the catalysts, it was observed that the catalyst with the Cu_2O/CuO molar ratio of 68/32 has the highest photocatalytic activity (i.e., the most efficient gas evolution under illumination). A theoretical study was carried out to understand the role of Cu_2O in the photocatalytic process. The catalyst surfaces were modelled using the Quantum Espresso Suit of software and the graphical user interface of the same "BURAI". Density functional theory calculations were conducted using Perdew-Burke-Ernzerhof exchange-correlation (PBE) ultra-soft pseudopotentials. The efficiency of adsorption of the molecules of interest, i.e., H_2O, CH_3OH, H_2 and CO_2, on Cu_2O (111) and CuO (111) surfaces was investigated by calculating the adsorption energies. The theoretical investigation revealed that hydrogen adsorption on Cu_2O (111) is ~49 times stronger than that on CuO (111). Also, the Cu_2O (111) surface is more hydrophilic than CuO (111). Formation of CuO (111) on Cu_2O (111) surface may impart the desired properties by minimizing the adsorption of H_2 and thereby minimizing its dissociation. This would have improved the photocatalytic activity of the Cu_2O (111)/CuO (111) composite surface.

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