Analysis of Data from Published Articles for Photocatalytic CO2 Reduction over Halide Perovskites

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Among all greenhouse gases accumulating in the atmosphere, carbon dioxide is the main reason of global warming[1]. Hence, extensive efforts have been made to develop environmentally friendly technologies that eliminate CO_2 emmisions. Photocatalytic CO_2 reduction, i.e. artificial photosynthesis, is one of the most promising strategies to convert the undesired CO_2 into valuable chemicals such as methane, methanol, carbon monoxide and hydrogen by means of solar energy[2]. In the search of an efficient photocatalyst, various semiconductors have been employed for CO_2 reduction processes; recently, halide perovskites have been explored as an appropriate candidate due to their tunable band gap, favorable light absorption capacity, and long carrier transport length as observed solar cell applications[3,4].

Halide perovskites are represented with a chemical structure of ABX_3, where A and B sites are cations and X is a halide anion[5]. The properties of halide perovskites photocatalysts can be tuned by composition engineering, doping or using co-catalysts. In this context, numerous experimental studies have been performed to design halide perovskite photocatalysts with excellent efficiency under optimum reaction conditions. The increasing interest on halide perovskite photocatalysts over time as seen in Figure 1 caused accumulation of data in literature, which can be analyzed by machine learning tools to identify the path that leads to improved photocatalytic performance.

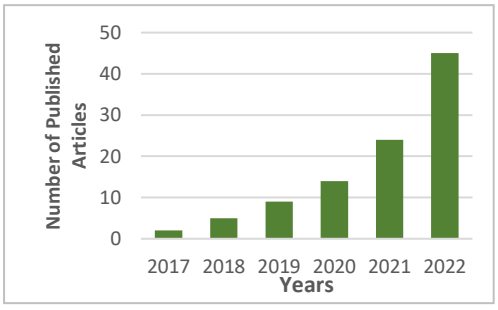

Figure 1. The Number of Published Articles on Photocatalytic CO_2 Reduction over Halide Perovskites

For this purpose, 115 articles published from 2017 to 2023 on photocatalytic CO_2 reduction over halide perovskites were studied to build a comprehensive database. The database consists of parameters such as perovskite type, crystal structure, particle size, band gap, catalyst preparation method, co-catalyst type and weight percent, light type, reaction phase, reaction medium and time. In addition, CO production rate was selected as output variable.

First, a simple descriptive statistics was used to identify the significant factors and major patterns in dataset to see their effects on production rate. Photocatalytic CO2 reduction reactions conducted in both liquid and gas phases. The analysis shows that performance of photocatalytic CO_2 reduction in liquid phase is better than that of in gas phase as it is evident from Figure 2. CO is the main product for both phases. Also, regardless of the reaction phase, halide perovskite photocatalysts favor gaseous products CO, CH_4, and H_2. In addition, the parameters such as perovskite composition, co-catalyst type, co-catalyst loading, and preparation methods directly are found to be effective in band gap, crystal structure, and hence performance of photocatalysts. Then, predictive models for CO production rate in both phases were developed using machine learning tools. The most influential variables for CO production were selected as descriptors for the models.

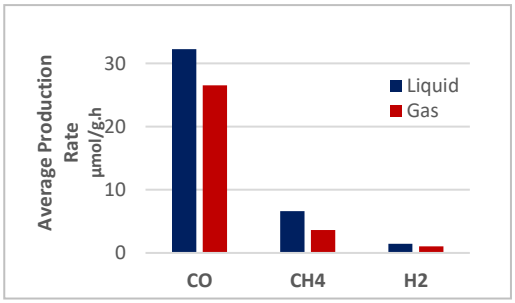

Figure 2. Average Production Rates for Products in Photocatalytic CO_2 Reduction over Halide Perovskites for Liquid and Gas Phase Processes.

References

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Beyza Yılmaz is currently a PhD Candidate in Department of Chemical Engineering at Boğaziçi University. Her research interests include solar energy, perovskites, perovskite solar cells, catalysis and photocatalytic carbon dioxide reduction technologies.

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