Photocatalytic CO_2 reduction

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As one of the major greenhouse gases, CO_2 emission has to be reduced for a sustainable world. While new and cleaner energy conversion technologies have been developed to cease the dependency to the fossil fuels, the effective technologies to convert the emitted CO_2 into more environmental friendly, and preferably economically valuable chemicals have been also investigated. Photoreduction of CO_2 using solar energy and water, as inspired by photosynthesis in plants, has been investigated extensively for this purpose in recent years. Figure 1 shows the increase in number of publications through years with the "photocatalytic CO_2 reduction" keyword in Web of Science (WOS) database [1]. When this technology becomes commercially available, it will be possible to produce valuable chemicals with a clean technology while reducing CO_2 emissions into the atmosphere.

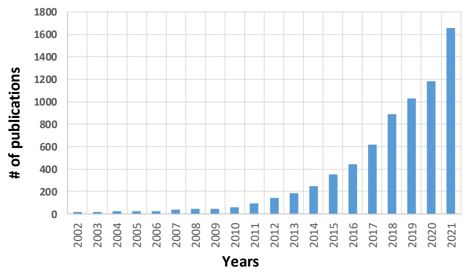

Figure 1. Publications on photocatalytic CO_2 reduction (based on WOS search in 13.4.2023 with the keyword of "photocatalytic CO_2 reduction" as *topic*)

The photoreduction of CO_2 can be carried out photoelectrochemically (using photoactive electrodes containing cocatalyst) or photocatalytically (using particulate photoactive semiconductors loaded by cocatalyst). Although the photoelectrochmical process has to be in liquid phase, the photocatalytic processes are performed in both liquid and gas phase conditions with different product distribution [2].

Photoreduction of CO_2 using solar energy is clearly quite appealing; however, there are several challenges to overcome for a successful commercialization of the process. For example, semiconductors with sufficient visible light activity are needed if the process is going to use solar irradiation; unfortunately, most of the available semiconductor are active under UV or have very low efficiency under visible light irradiation. Additionally, the semiconductor to be used should be cheap, stable and harmless to the human health and environment. Consequently, one of the main research direction in the field is to find new and better semiconductors by searching among natural materials, modifying existing semiconductors or synthesizing completely new materials. Indeed, from simple metal oxides to metal organic frameworks (MOFs) and halide perovskites, various materials have been studied for this purpose. Similarly, effective cocatalysts to improve the charge separation and reaction rate are also investigated.

Due to the complexities in the process and challenges in finding suitable semiconductors and cocatalysts, the experimental works has to be supported by computational tools to reduce the search space, and to direct the experimental studies to the most the promising conditions. Two classes of computational tools have been used for this purpose as in other similar research fields: molecular modeling (mostly DFT based) and machine learning. While the molecular modeling is used to determine the suitability of physical and chemical properties of the new materials, the machine learning allows for the screening of larger number of alternatives by predicting the properties or performance of completely new materials using information from already known alternatives. This two approach are often used together through computational material databases like Material Project, OQMD, AFLOWLIB, and Computational Material Repository containing physical and chemical properties of hundreds of thousands materials. Data from these databases, together with experimental data accumulated on the subject through the years, create a big opportunity to learn from the past experience via machine learning and use this information to discover, select or analyze materials with potential as semiconductor or cocatalyst.

To sum up, although significant challenges are still ahead for the successful commercialization of CO_2 photoreduction, there are also significant development to speed up the progress in the field.

References

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