Engineering and physical science

VCU TechTransfer and Ventures
Office of the Vice President for Research and Innovation

CO_2 Hydrogenation Method

Utilizing Ligated Metal Chalcogenide Clusters as Catalysts to Control Reaction Rates

The greenhouse effect is a phenomenon that causes harmful global environmental changes due to increasing CO_2 levels in the earth's atmosphere. As such, reducing the levels of CO_2 through means of capturing the CO_2 is a potential solution to mediate the greenhouse effect. Currently, porous or mesoporous absorbents are utilized to capture CO_2. However, upscaling this process is often impractical due to the costly CO_2 storage and transportation. Thus, researchers at VCU have developed an effective alternative to reducing atmospheric CO_2 levels by capturing and converting it into useful bi-products, such as formic acid, via novel ligated metal chalcogenide clusters.

The technology

Converting CO_2 to formic acid without an effective catalyst is challenging as CO_2 is inherently inert. The use of VCU's novel metal chalcogenide cluster as a catalyst for CO_2 hydrogenation contains a unique capability to alter its energy demand based on the attached ligand (i.e., the barrier height can be controlled by varying the number/type of attached ligands) (Figure 1 and Figure 2). For example, the un-ligated metal chalcogenide cluster produced significantly low barrier heights ranging from 0.3-0.4 electron volts (eV) compared to conventional catalysts. By selectively controlling the ratio of attached acceptor and donor ligands to the metal chalcogenide cluster, one can adjust the barrier heights for CO_2 hydrogenation in a stepwise manner. For instance, by attaching only three specific ligands to the cluster, one of the CO_2 hydrogenation barriers can be reduced to as low as 0.12 eV that will allow rapid thermochemical conversion of CO_2.

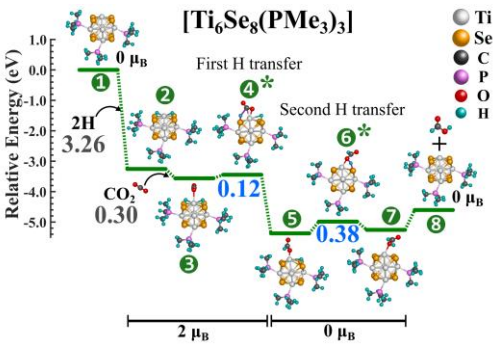

Figure 1. CO_2→HCOOH reaction pathway on $[Ti_6Se_8(PMe_3)_3]$ metal chalcogenide cluster.

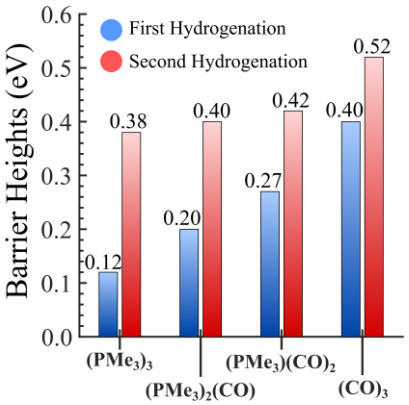

Figure 2. The relative trend of barrier heights for both hydrogenation steps on four ligated clusters.

Benefits

- Low energy CO_2 capture catalyst
- Controllable reaction rate

Applications

- Hydrogen energy storage
- CO_2 capture
- Formic acid production

Patent status:
Patent pending: U.S. and foreign rights are available.

License status:
This technology is available for licensing to industry for further development and commercialization.

Category:
Engineering and physical science

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