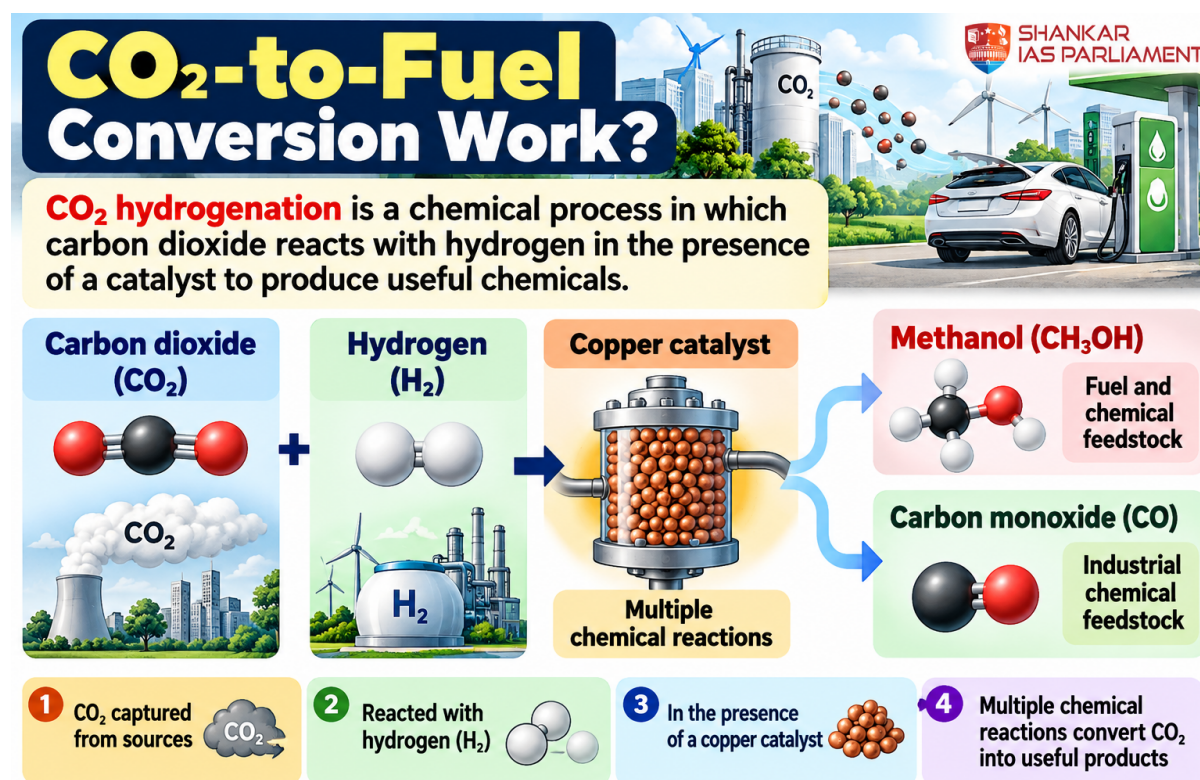


AI-Based Model for CO₂-to-Fuel Conversion

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Why in News?

Researchers at the IISc, Bengaluru, developed a computational framework that maps 9,389 elementary chemical reactions for converting CO₂ into useful fuels and chemicals.



Key Findings

- The researchers expanded the initial database from 152 to 9,389 reactions.
- The network includes 105 chemical species present on the catalyst surface.
- A model limited to 152 reactions predicted formic acid as the main product and underestimated CO₂ conversion.
- The expanded model predicted a 40-fold increase in CO₂ conversion and identified methanol and carbon monoxide as major products, consistent with experimental results.
- The model also identified a less conventional pathway where molecular hydrogen (H₂) transfers hydrogen directly to intermediates without first splitting into individual

atoms.

Technologies Used

- **Quantum-mechanical simulations** - Estimate reaction energies and barriers based on quantum mechanics.
- **Machine learning (ML)** - Predicts energy barriers for additional reactions to reduce computational effort.
- **Automated reaction mapping** - Identifies potential reactions among chemical species to build a comprehensive reaction network.

Significance

- **Improved accuracy** - This approach reduces errors by ensuring that potentially important reactions are not excluded.
- **Catalyst design** - It may assist in developing catalysts that favor pathways leading to methanol.
- **Carbon utilisation** - This framework supports research focused on converting captured CO₂ into valuable products.
- **Wider applications** - The framework can also be applied to CO₂ reduction with other catalysts, as well as to nitrogen reduction and water splitting.

Reference

[TOI | CO₂ Hydrogenation](#)

