NH3 Synthesis using a Stable Electride C12A7 as Electron Donor and Reversible Hydrogen Store

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1. Present Industrial NH_3 Synthesis

- 160 million tons of NH3 are produced each year through industrial processes at high temperature and high pressure.
- Iron based catalysts (Haber-Bosch method) or Ru metal particles dispersed on a support material in the industrial processes are used.

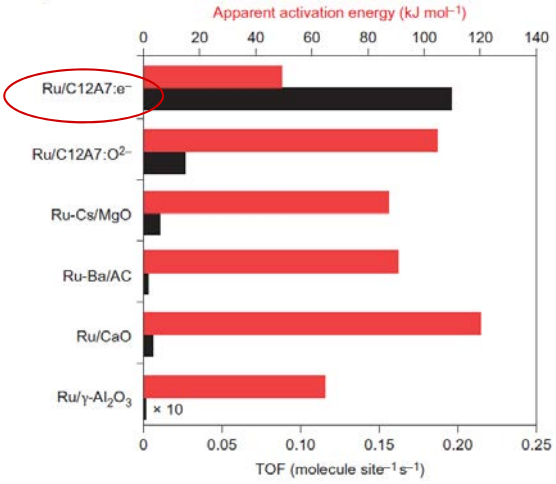
Haber-Bosch method; $N_2 + H_2 \xrightarrow{Fe} NH_3$ (400-600 ℃, 20- 40 MPa)

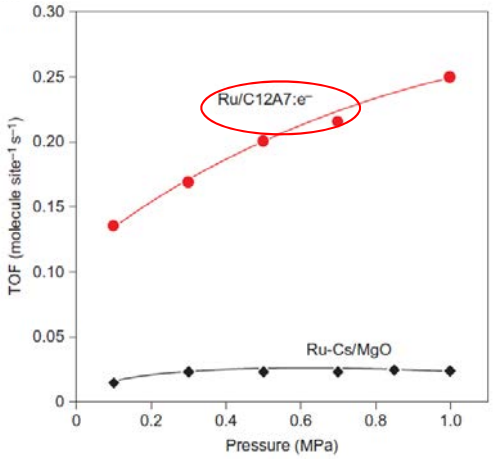
- The determining step is the **dissociation of both N_2 and H_2** on the metallic catalyst surface, and it is also important for the surface not to become covered by H_2 blocking active sites for N_2 dissociation (→**H_2 poisoning**).
- These processes consume a great deal of energy (around 1-2% of worldwide energy apply).

A novel supported Ru catalyst promotes N_2 & H_2 dissociation but suppresses H_2 poisoning, which will bring big energy savings.

2. Catalytic Performance of Ru-loaded C12A7 Electride for NH_3 Synthesis

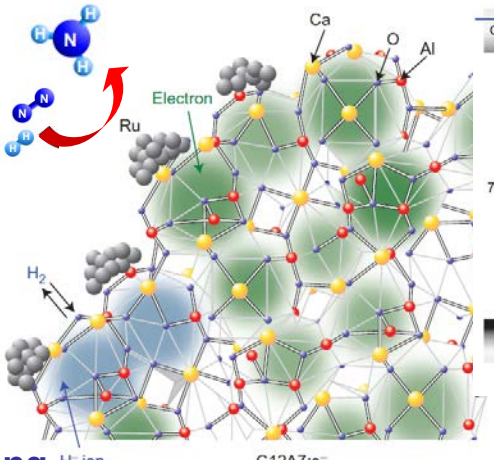
- Ru-loaded C12A7:e catalyst activity (TOF) shows one order magnitude greater than some current Ru catalysts. And also the catalyst exhibits the smallest activation energy.

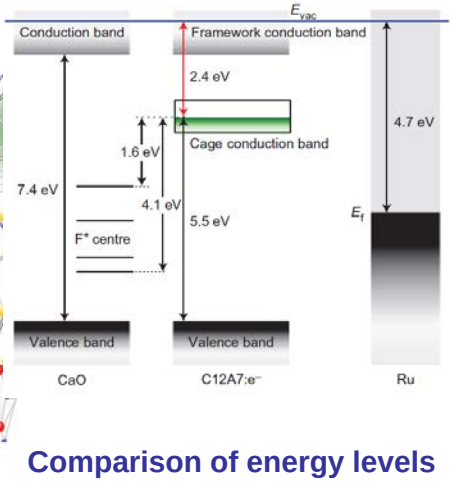




3. Schematic Model of Ru-loaded C12A7 Electride in NH_3 Synthesis

- N≡N bond becomes weakened by electron donating from C12A7;e to the N_2 anti-bonding orbital.
- The C12A7;e also has the role of H_2 scavenger, and transforms H atom to hydride which is reversibly incorporated into the C12A7 nanocages.





Comparison of energy levels

4. Patent available for licensing

Patent No. : WO 2012/077658

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