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AMBHER

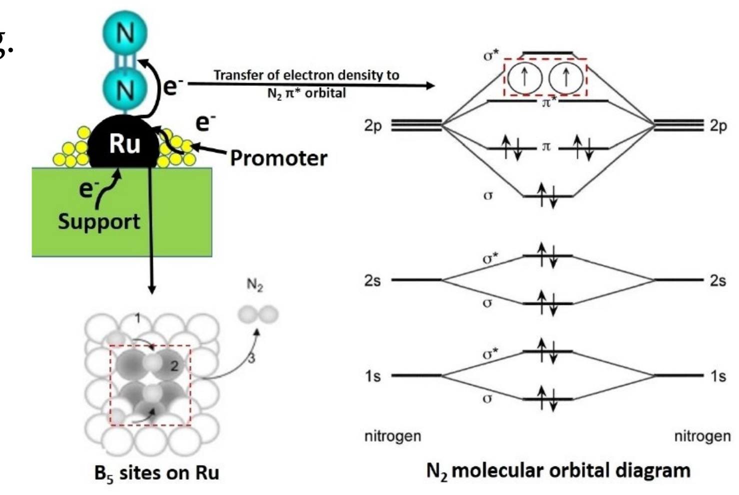
Transition metal nanoparticle-based catalysts for ammonia synthesis

María Dolores Seva[1], Elena Vicente[1], Simona Somacescu[2], David Catalán Martinez[1], Jesús Ara[1], Álvaro Represa[1], José Manuel Serra[1], María Balaguer[1], Sonia Escolástico[1].

[1]Energías Renovables/Instituto de Tecnología Química/CSIC/Universitat Politècnica de València, Valencia, España
[2]Department of Catalysis and surface Chemistry/Institute of Physical Chemistry/Bucharest, Romania

Introduction

- Industrial production of NH_3 → Haber-Bosch process contributing 1-2% to global anthropogenic CO_2 emissions[1].
- The HB process involves → use of Fe-based catalysts and extreme operating conditions of P and T→ cost-effective NH_3 synthesis catalysts are still lacking at moderate conditions.
- Ru-based catalysts → production rates of NH_3 have not yet compensated for the high costs of this metal. In addition, they often suffer from H_2 poisoning.
- Addition of electron donors[2] → allows e⁻ transfer to the Π* orbitals of N_2.

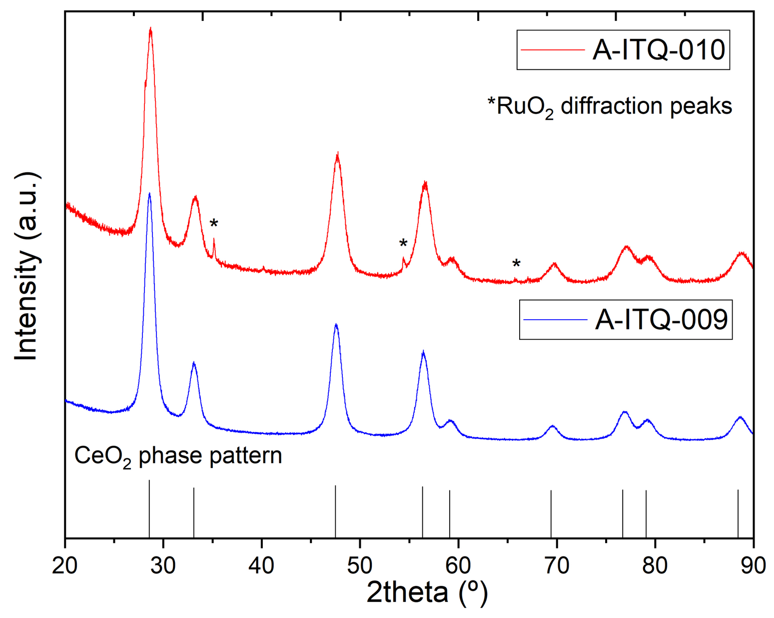


(1) *Annual Review of Chemical and Biomolecular Engineering 2020, 11, 503-521*
(2) *ChemCatChem* 2020, 12, 5838–5857

Objectives

- Reduction of environmental impact
  - Minimize CO_2 emissions related to ammonia production
- Optimization of energy efficiency:
  - Develop catalysts that require lower energy consumption by reducing the need for high pressures and temperatures in the NH_3 synthesis process. Reach high NH_3 productions at T< 250ºC and P < 20 bar
- Study of stability and durability:
  - Evaluate the long-term stability and resistance to H_2 poisoning of transition metal nanoparticle-based catalysts.

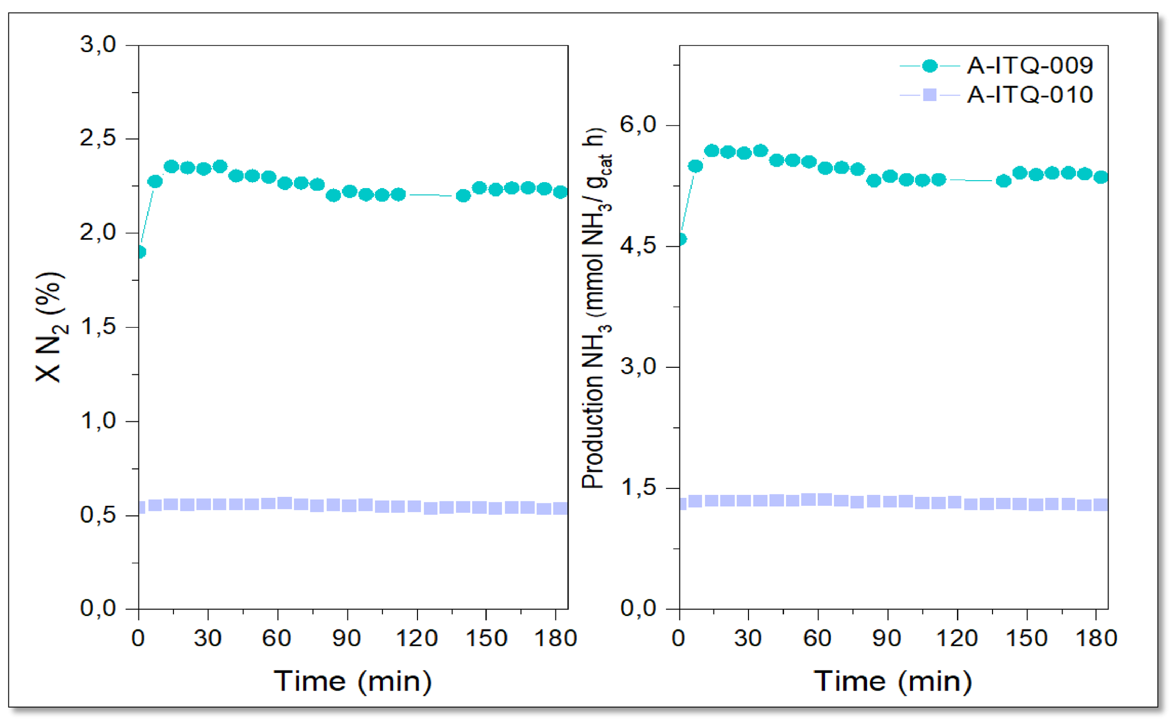
Results



X-ray diffraction patterns

A-ITQ-009: only cubic fluorite diffraction peaks are detected, suggesting high Ru dispersion

A-ITQ-010: additional RuO_2 peaks are observed, suggesting Ru agglomeration



NH_3 production results for A-ITQ-009 and A-ITQ-010

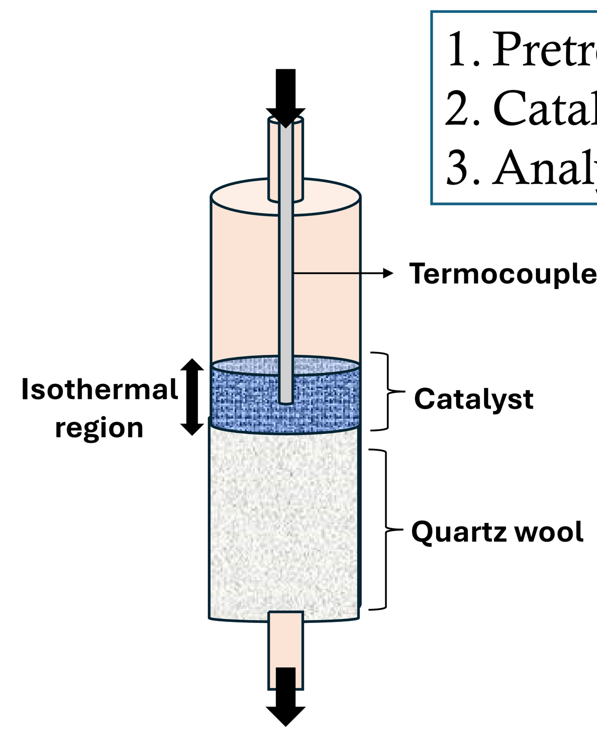
H_2:N_2=3 T=400 ºC P=30 bar,
WHSV (mL· g⁻¹· h⁻¹)=9.000
Pretreatment of 60 ml/min H2 at 550ºC 1h

Sample	BET area (m^2/g)
A-ITQ-009	108
A-ITQ-010	91

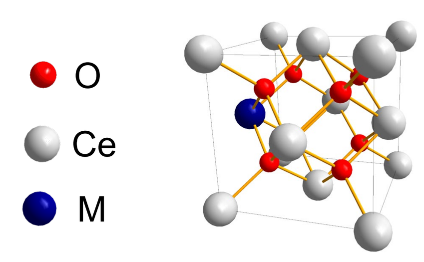
N_2 adsorption Type IV isotherm with a hysteresis loop H1 suggesting a mesoporous structure

Experimental Procedure

1. Pretreatment (H_2, 550º C)
2. Catalytic test
3. Analysis of results (GC)



Catalyst → transition metal nanoparticles supported on oxides with redox properties.



Sample	Catalyst	Synthesis method	Tcalcination (ºC)
A-ITQ-009	Ru-doped ceria	Hydrothermal	550
A-ITQ-010	Ru-Ni-doped ceria		

Conclusions

- A-ITQ-009 shows higher catalytic activity that may be linked to an appropriate metal loading and a homogeneous distribution of Ru particles compared to A-ITQ-010.
- The catalytic results show high N_2 conversion and no deactivation after over 180 minutes of, indicating good stability of the catalyst under the studied conditions.
- In conclusion, promising Ru-based catalysts were developed for the NH_3 synthesis reaction at moderate conditions.
- However, there is still a need for further research and improvement of these catalysts to make them competitive with those currently used in the HB process.

Acknowledgements

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