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# High-Performance Rh@MgO Catalysts for Complete Dehydrogenation of Hydrazine Borane: A Comparative Study

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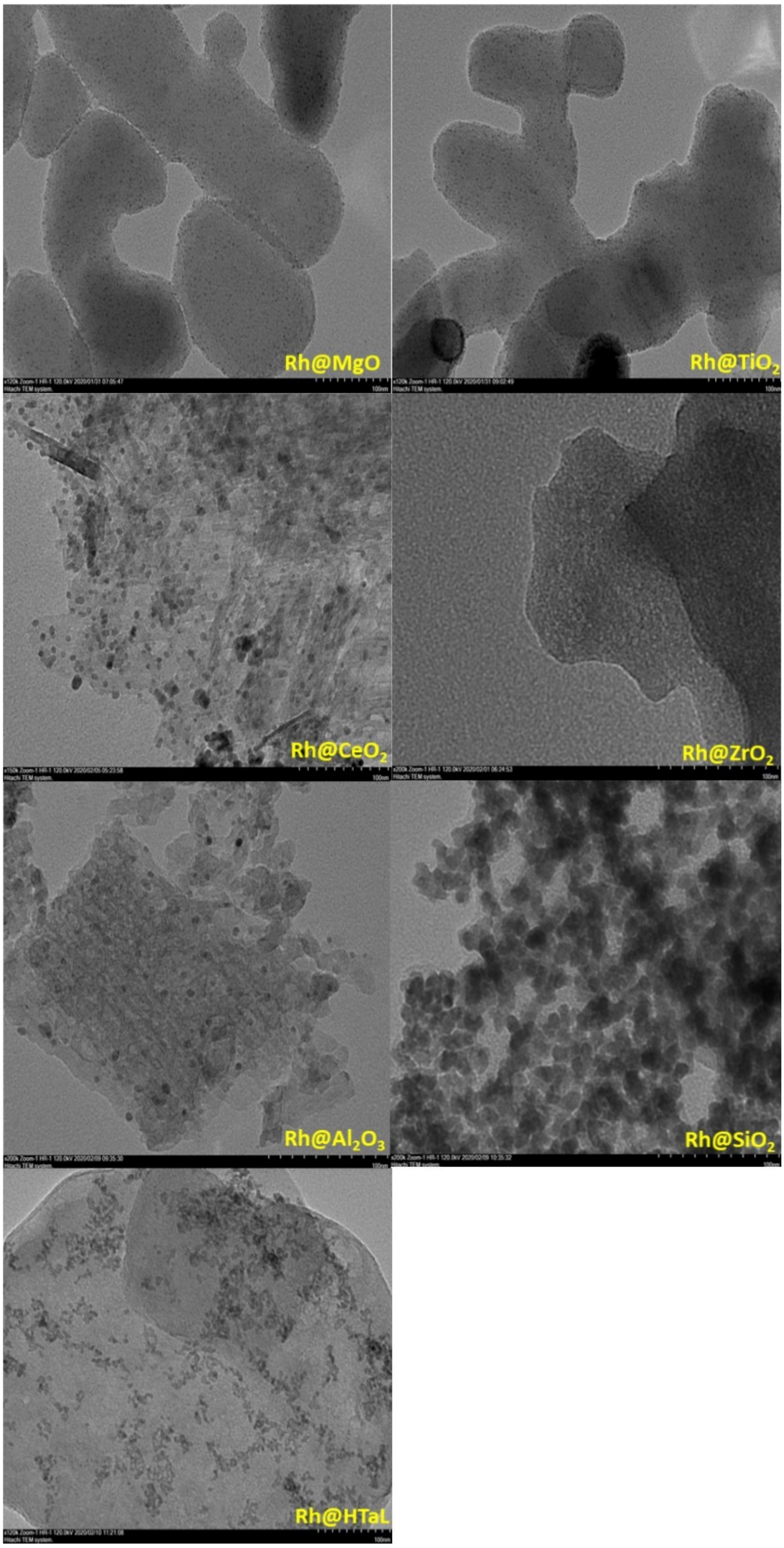


Figure S1. TEM images of monometallic Rh(0) nanoclusters immobilized on different support materials.

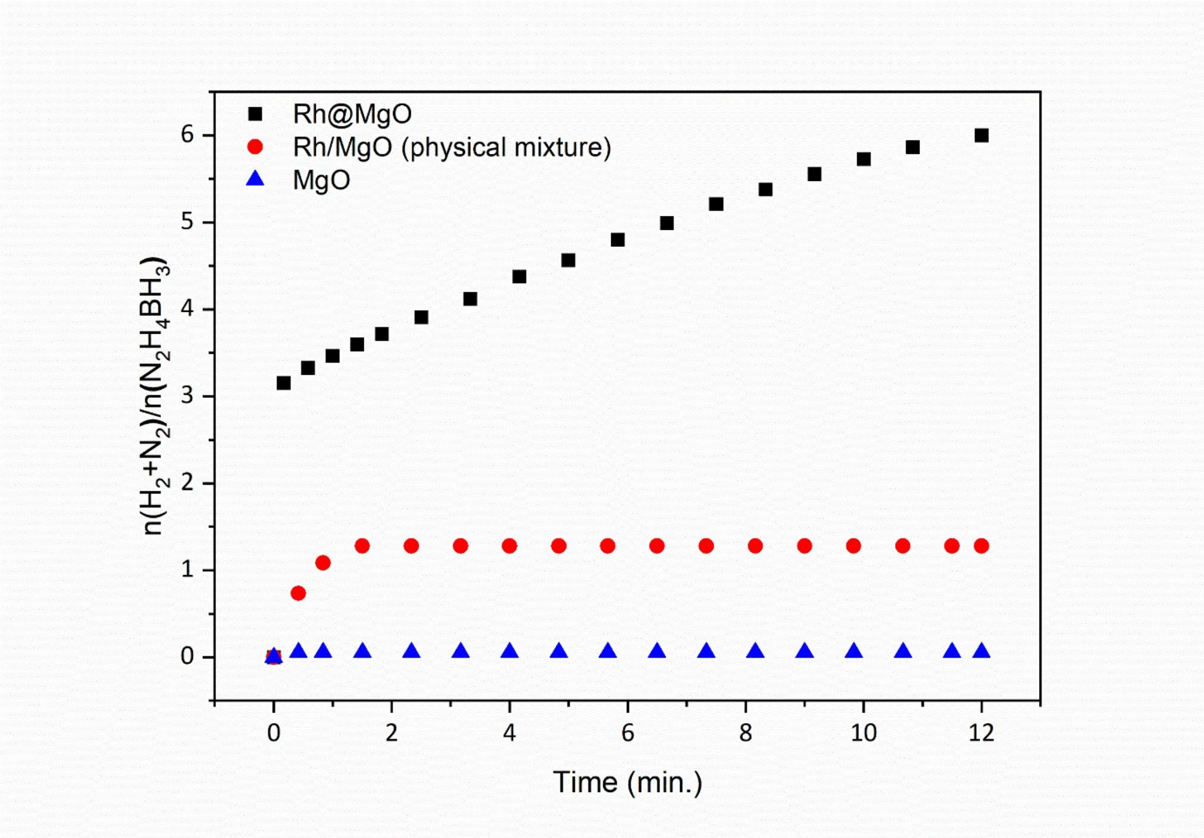


Figure S2. Mole ratio of generated gas ($H_2$ + $N_2$)/HB versus time graph for the Rh@MgO, Rh/MgO (physical mixture) and MgO-catalyzed dehydrogenation of aqueous HB.

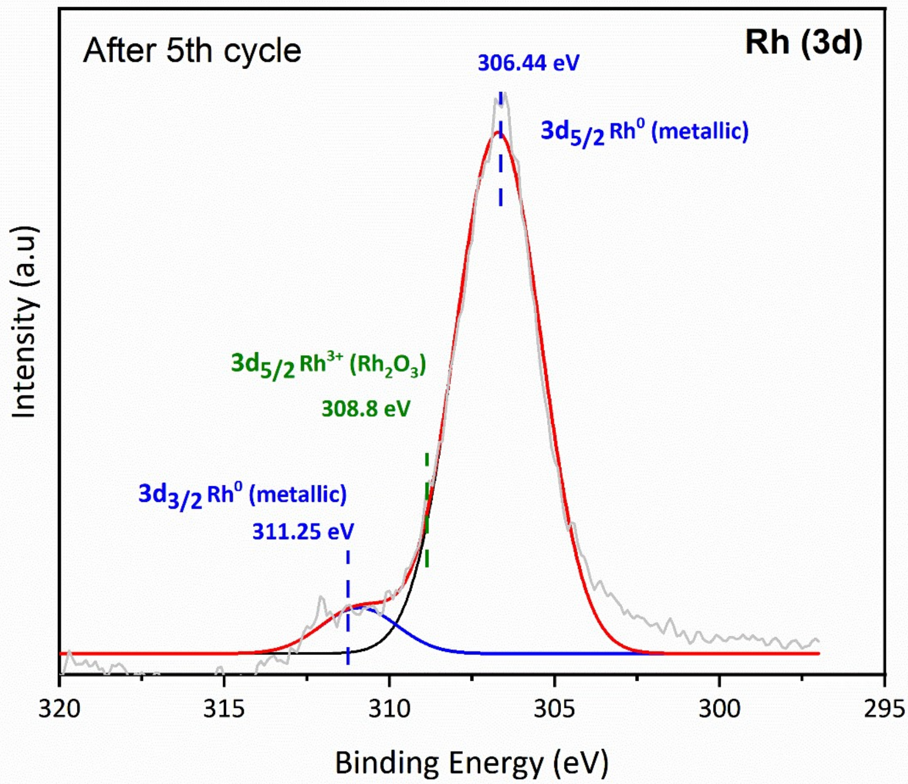


Figure S3. Rh (3d) XPS spectra of Rh@MgO after the 5th reuse cycle, showing the preservation of the metallic Rh structure with minimal shifts, indicating catalyst stability over multiple cycles.

Table S1. Heterogeneous catalysts tested for the complete degradation reaction of hydrazine borane ($N_2H_4BH_3$) in water and capable of conversion.

| No | Catalyst | Temperature (K) | TOF ($h^{-1}$) | Ref. |
|---|---|---|---|---|
| 1 | $Ni@RhNi/Al_2O_3$ | 323 | 72 $h^{-1}$ | [1] |
| 2 | $Rh_{0.8}Ni_{0.2}@CeO_x/rGO$ | 323 | 667 $h^{-1}$ | [2] |
| 3 | $Ni_{0.9}Pt_{0.1}$/Graphene | 323 | 242 $h^{-1}$ | [3] |
| 4 | $Ni_{0.9}Pt_{0.1}/CeO_2$ | 323 | 234 $h^{-1}$ | [4] |
| 5 | $Ni_{0.9}Pt_{0.1}$/MIL-101 | 323 | 1515 $h^{-1}$ | [5] |
| 6 | $NiIr/Cr_2O_3$ | 323 | 248 $h^{-1}$ | [6] |
| 7 | $Ni\text{-}MoO_x/BN$ | 323 | 600 $h^{-1}$ | [7] |
| 8 | $Ni_{0.5}Fe_{0.5}\text{-}CeO_x$/MIL-101 | 323 | 352 $h^{-1}$ | [8] |
| 9 | $Cu_{0.4}Ni_{0.6}Mo$ | 323 | 108 $h^{-1}$ | [9] |
| 10 | $Ni_{0.75}Ir_{0.25}/La_2O_2CO_3$ | 323 | 1250 $h^{-1}$ | [10] |
| 11 | $Rh_{0.5}(Mox)_{0.5}$ | 323 | 2000 $h^{-1}$ | [11] |
| 12 | $Ni_{0.22}@Ir_{0.78}$/OMS-2 | 323 | 2590 $h^{-1}$ | [12] |
| 13 | Rh@MgO | 323 | 2005 $h^{-1}$ | This Work |

**Determination of Average Turnover Frequency (TOF) Values**

The activity values in this report are not corrected for the number of exposed surface atoms; that is, the values given are lower limits.

For Rh@MgO catalyst; mol (Rh) = 1.496 µmol, mol (HB) = 1 mmol , Rh@MgO catalyst provides 6 moles equiv. gas generation at t = 12 min.

TOF(average) = moles of product / moles of catalyst × time (where 100 % conversion was achieved)

TOF(average) = ($6\times10^{-3}$ mol) / ($1,496\times10^{-5}$ mol) × (12/60 h)

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