Electronic Supplementary Material (ESI) for Faraday Discussions.

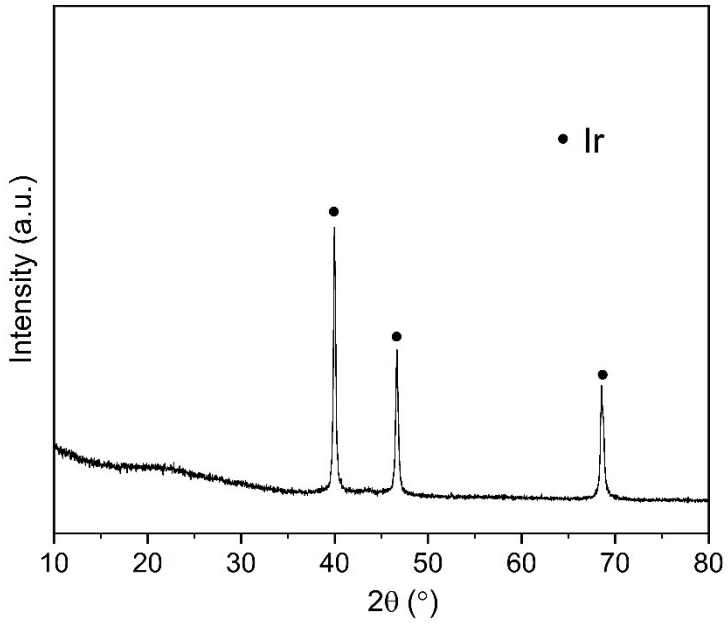

Figure S1. XRD patterns of the as-prepared Ir metal. The reference pattern code of Ir is 00-046-1044.

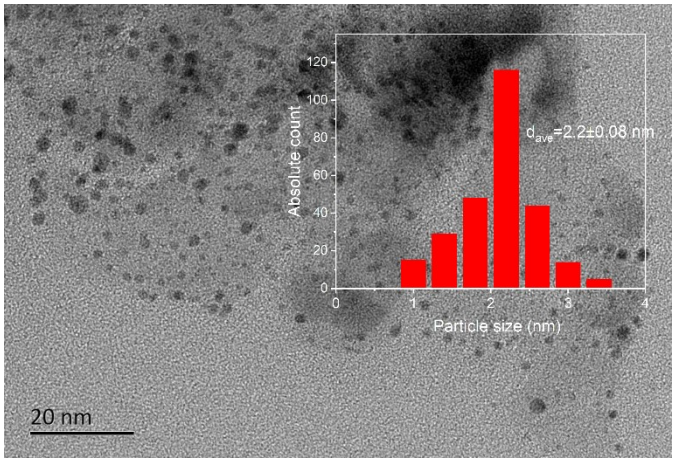

Figure S2. TEM image of the hydrogenated LiH-Ir/MgO catalyst. The inset picture shows the corresponding particle size distribution.

Table S1. Kinetic parameters of LiH-Ir/MgO catalyst and the conventional Ru and Fe catalysts.

Catalyst	Reaction order[a]			E_a (kJ mol^{-1})
	$\alpha(NH_3)$	$\beta(N_2)$	$\gamma(H_2)$	
LiH-Ir/MgO[a]	-0.65	1.27	-0.36	53.4 (300-400 ºC)
Cs-Ru/MgO[b]	-0.09	1.01	-0.82	112.4 (250-325 ºC)
Ru/MgO[b]	-0.24	1.12	-0.86	94.8 (250-325 ºC)
KM1[c]	-1.50	0.90	2.20	70 (320-400 ºC)

[a]Reaction orders of N_2, H_2, and NH_3 of LiH-Ir/MgO were measured at 350 ºC and 10 bar;

[b]Reaction orders of N_2, H_2, and NH_3 of Cs-Ru/MgO or Ru/MgO were measured at 300 ºC and 1 bar (Chen et al.[1]);

[c]Reaction orders of N_2, H_2, and NH_3 of KM1 were measured at 300 ºC and 10 bar (Chorkendorff et al.[2]).

References

1. Q. Wang, J. Pan, J. Guo, H. A. Hansen, H. Xie, L. Jiang, L. Hua, H. Li, Y. Guan, P. Wang, W. Gao, L. Liu, H. Cao, Z. Xiong, T. Vegge and P. Chen, *Nat. Catal.*, 2021, **4**, 959-967.
2. S. Hagen, R. Barfod, R. Fehrmann, C. J. H. Jacobsen, H. T. Teunissen and I. Chorkendorff, *J. Catal.*, 2003, **214**, 327-335.