

Supplementary Material

Enhancing the Activity of Supported Rhenium-catalyzed Cross-Metathesis of Ethene and 2-Butene *via* promotion of boron

Yibo Yang,^{‡abc} Gaolei Qin,^{‡abc} Anping Yin,^{abc} Yuhang Cai,^{abc} Ziyu Zhou,^{abc} Nengfeng Gong,^{abc} Xiangjie Zhang,^{abc} Tao Yan,^{abc} Gengzhe Song,^b Xiaodong Sun,^b Hongliu Wan,*^b Yong Yang,^{abc} Yongwang Li^{abc} and Zhi Cao *^{abc}

^a. State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, 030001, China

^b. National Energy Center for Coal to Liquids, Synfuels China Co., Ltd., Beijing, 101400, China

^c. University of Chinese Academy of Sciences, Beijing, 100049, China

* Corresponding author

‡ Yibo Yang and Gaolei Qin contributed equally to this work.

E-mail: wanhongliu@synfuelschina.com.cn (Hongliu Wan), caozhi@sxicc.ac.cn (Zhi Cao).

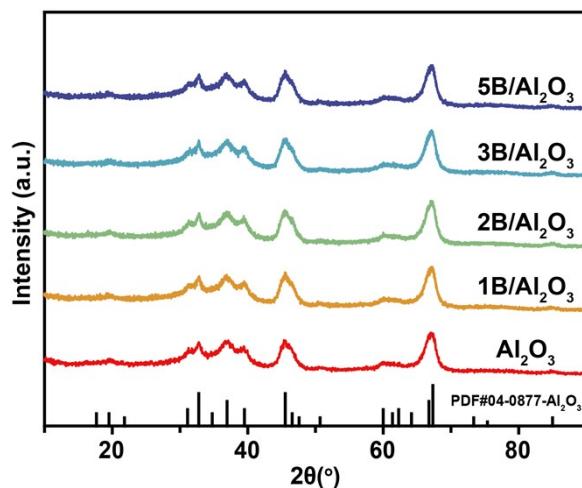


Fig. S1. XRD patterns of xB/Al₂O₃ supports.

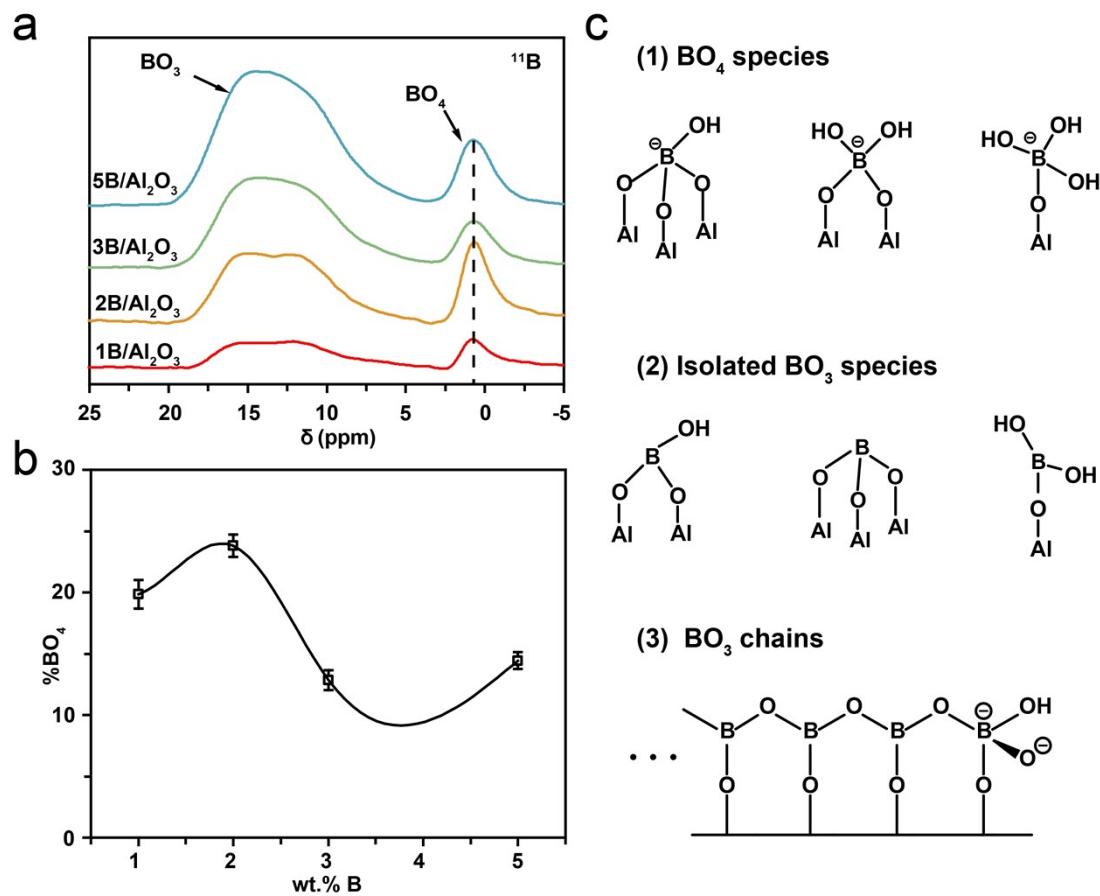


Fig. S2. (a) ^{11}B MAS-NMR spectra illustrating the spectral region for the central transitions for the $x\text{B}/\text{Al}_2\text{O}_3$ supports. (b) The fraction of BO_4 species determined as $I(\text{BO}_4)/\{I(\text{BO}_4) + I(\text{BO}_3)\}$, as a function of the total boron content for the $x\text{B}/\text{Al}_2\text{O}_3$. (c) Schematic structures of BO_x species on an alumina surface.

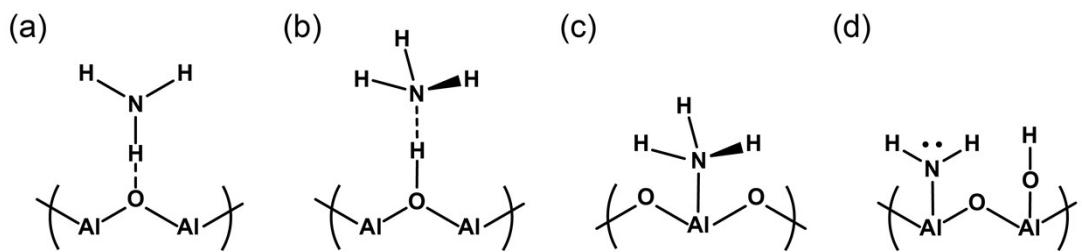


Fig. S3. Ammonia adsorption modes on acid sites: (a) Ammonia forms hydrogen bonds with surface oxygen atoms through its hydrogen (H) atoms. This is the weakest interaction mode. (b) Proton transferred from the surface hydroxyl group acting as a Brønsted acid site to the adsorbate. (c) The nitrogen atom of NH_3 coordinates with aluminum ions, which act as Lewis acid sites. (d) NH_3 undergoes dissociative adsorption, simultaneously forming a hydroxyl group, which stabilizes NH_3 on the solid surface.

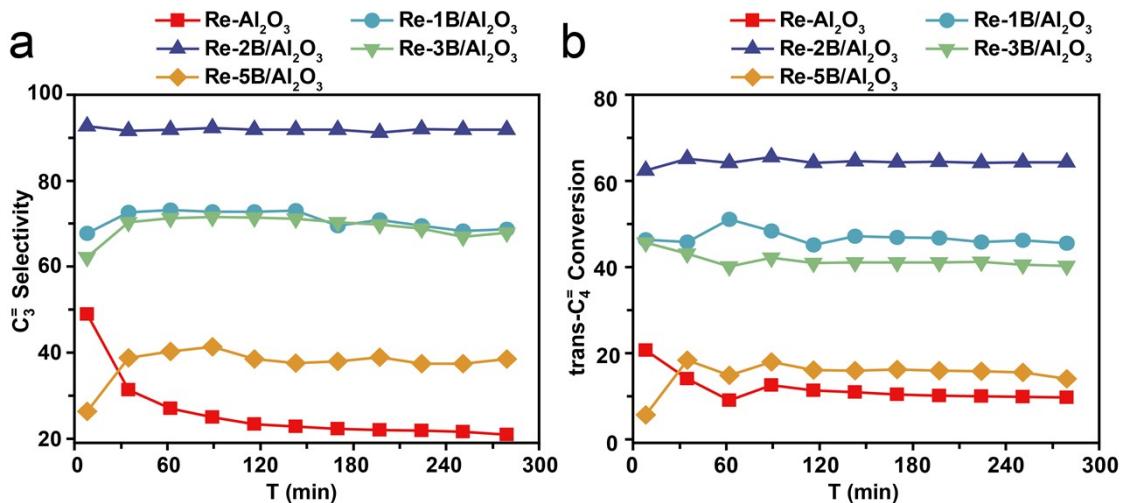


Fig. S4. (a) Time-on-stream selectivity of propene for Re-xB/Al₂O₃ catalyzed metathesis of C₂⁼ and trans-2-C₄⁼. (b) Time-on-stream conversion of 2-Butene for Re-xB/Al₂O₃ catalyzed metathesis of C₂⁼ and trans-2-C₄⁼.

Table S1. Comparison on the catalytic performance of metathesis over different rhenium catalysts.¹⁻⁵

Catalyst	Substrates	TOF/h ⁻¹	Reference
Re-2B/Al ₂ O ₃	ethane and 2-butene	96.2	This work
Re-SiO ₂ -Al ₂ O ₃	ethane and 2-butene	64.1	<i>ACS Catal.</i> , 2021, 11, 3530–3540
Re-ZSM-5	propene	12.2	<i>ACS Catal.</i> , 2021, 11, 2412–2421
Re/AlMCM-41	ethane and 2-butene	46.8	<i>Catalysts.</i> , 2022, 12, 188.
Re-SiO ₂ -Al ₂ O ₃ -Cl	1-octene	10	<i>J. Catal.</i> , 2008, 258, 61-70. <i>Microporous</i>
Re/meso-Al ₂ O ₃	1-octene	39.7	<i>Mesoporous Mater.</i> , 2004, 74, 93-103.

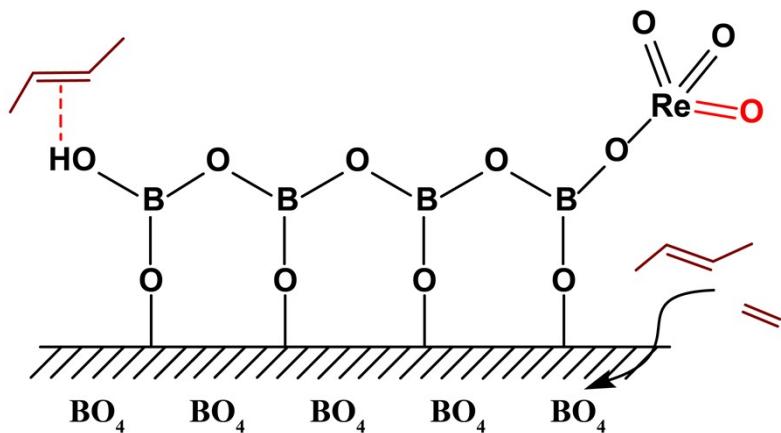


Fig. S5. The illustrative diagram on the $\text{ReO}_x\text{-B}$ sites with high boron loading.

Notes and references

1. P. Zhao, L. Ye, G. Li, C. Huang, S. Wu, P.-L. Ho, H. Wang, T. Yoskamtorn, D. Sheptyakov, G. Cibin, A. I. Kirkland, C. C. Tang, A. Zheng, W. Xue, D. Mei, K. Suriye and S. C. E. Tsang, *ACS Catal.*, 2021, **11**, 3530-3540.
2. B. Zhang, S. Lwin, S. Xiang, A. I. Frenkel and I. E. Wachs, *ACS Catal.*, 2021, **11**, 2412-2421.
3. M. Felischak, T. Wolff, L. Alvarado Perea, A. Seidel-Morgenstern and C. Hamel, *Journal*, 2022, **12**.
4. P. C. Bakala, E. Briot, Y. Millot, J.-Y. Piquemal and J.-M. Brégeault, *J. Catal.*, 2008, **258**, 61-70.
5. T. Oikawa, T. Ookoshi, T. Tanaka, T. Yamamoto and M. Onaka, *Microporous Mesoporous Mater.*, 2004, **74**, 93-103.