

Electronic Supplementary Information (ESI) for

**High NH₃-SCR reaction rate with low dependence on O₂ partial pressure
over Al-rich Cu-*BEA zeolite**

Yusuke Ohata,^a Takeshi Ohnishi,^a Takahiko Moteki^{a, b} and Masaru Ogura^{*a, b}

a. Institute of Industrial Science, The University of Tokyo, Komaba, Meguro, Tokyo 153-8505, Japan.

E-mail: oguram@iis.u-tokyo.ac.jp

b. Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, Katsura, Kyoto 615-8520, Japan

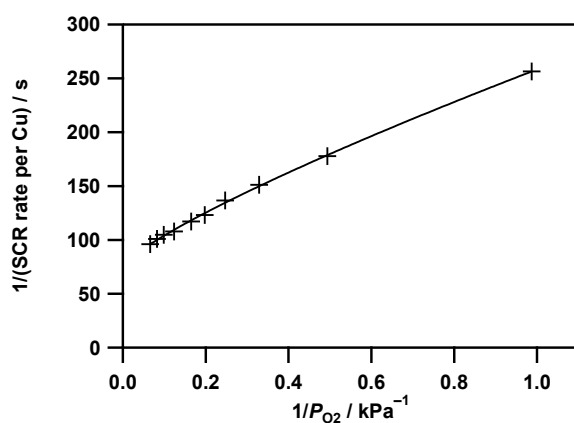


Figure S1. A plot for Langmuir equation over the reference Cu-SSZ-13 catalyst when the SCR rate was expressed by a function of P_{O_2} . This plot was expressed by a Lngmuir-Freundlich equation^[S1] with P_{O_2} order of 0.81.

Lngmuir-Freundlich equation:

$$\text{SCR rate per Cu} / \text{s}^{-1} = [a \times P_{O_2}^x / (1 + a \times P_{O_2}^x)]$$

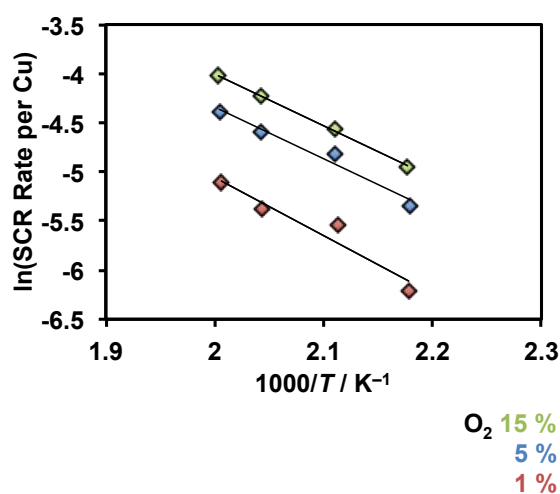


Figure S2. The Arrhenius plots around 473 K under several P_{O_2} reaction condition over the reference Cu-SSZ-13 catalyst.

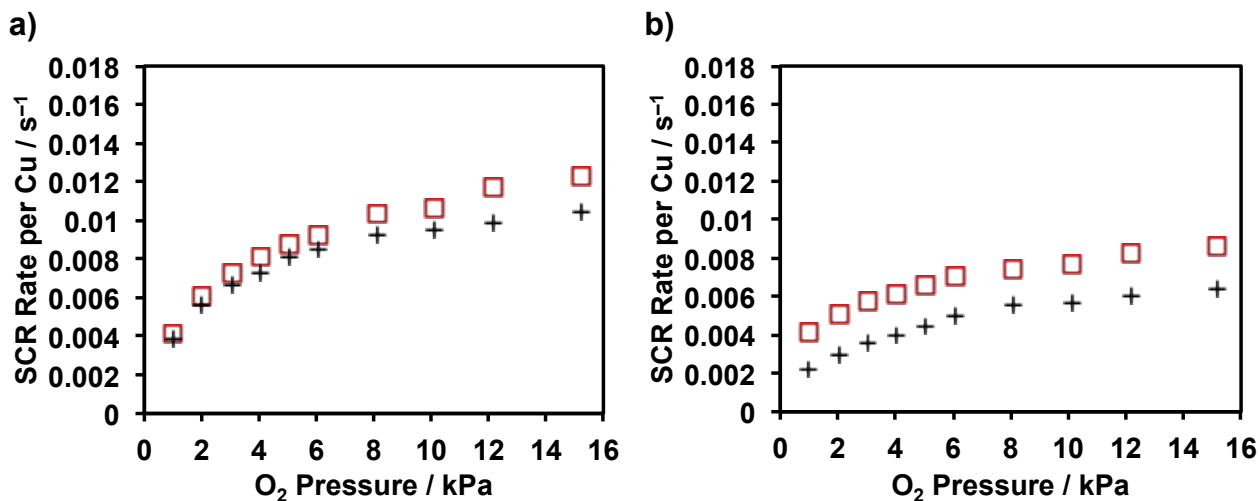


Figure S3. The dependence of NH_3 -SCR rate per Cu at a) 473 K and b) 460 K on O_2 pressure over the Cu-*BEA zeolite catalyst with several Cu density in micropores at $0.76 \text{ (1000 \AA}^3)^{-1}$ (red square symbol) and the reference Cu-SSZ-13 catalyst (the cross symbol).

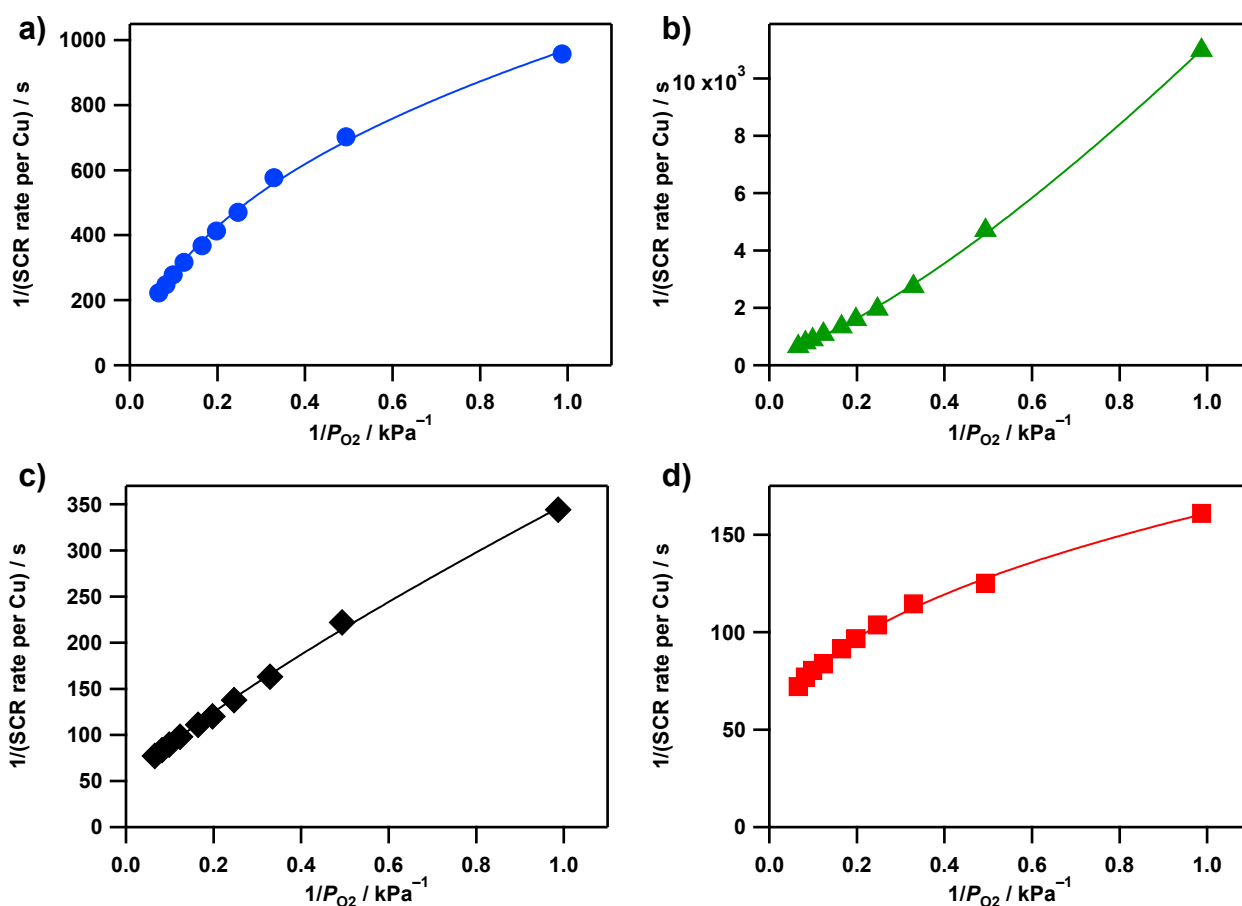


Figure S4. The plots for Langmuir equation over the a) Cu-MOR (M1), b) Cu-MFI (Z1), c) Cu-CHA (C3), and Cu-*BEA (B1) catalyst when the SCR rate was expressed by a function of P_{O_2} . These plots were expressed by the Lngmuir-Freundlich equation^[S1] with P_{O_2} order of 1.34, 0.40, 0.82, 0.42, respectively.

Table S1. The ion-exchange level and Cu density in micropores of the Cu ion-exchanged zeolite samples acquired in this study.^[S2,S3]

Entry.	Parent	Cu Ion-Exchange Level ^(a) / %	Na Ion-Exchange Level ^(b) / %	Cu Density in micropores ^(c) / (1000 Å ³) ⁻¹ [S2]
B12		13	88	0.76
B13		21	88	1.2
B14	Na-*BEA	30	74	1.7
B1	Si/Al = 5.6	39	66	2.2
B2		57	50	3.2
B5		92	17	5.2
Z1	Na-MFI	33	69	2.4
Z3	(Si/Al = 11.9)	78	31	5.7
Z12		101	0	7.4
M1	Na-MOR	36	72	2.5
M3	(Si/Al = 9)	64	47	4.4
M6		87	31	6.0
C1	Na-CHA	9.3	62	0.51
C3	(Si/Al = 6.9)	29	45	1.6
C5		62	0	3.4
C905	Na-CHA	64	21	2.2
	(Si/Al = 9)			

(a) Cu Ion-exchange level / % = (amount of Cu)/(amount of Al) × 200

(b) Na Ion-exchange level / % = (amount of Na)/(amount of Al) × 100

(c) Cu density in micropores / (1000 Å³)⁻¹ = (Cu/Al) × 1/(Si/Al + 1) × (T/1000 Å³)/((accessible volume / %)/100)

Reference

- [S1] D. M. Ruthven, *Principles of Adsorption and Adsorption Processes*, John Wiley & Sons, New York, The United States, 1984, 108.
- [S2] Y. Ohata, T. Nishitoba, T. Yokoi, T. Moteki and M. Ogura, *Bull. Chem. Soc. Jpn.*, 2019, **92**, 1935.
- [S3] Y. Ohata, H. Kubota, T. Toyao, K. Shimizu, T. Ohnishi, T. Moteki and M. Ogura, *Catal. Sci. Technol.*, 2020, *in press*. DOI: 10.1039/D0CY01838D