

In situ Ga K-edge XANES study of Ga-exchanged zeolites at high temperatures under different atmospheres including vacuum, CO, and pressurized H₂

Mengwen Huang¹, Tetsuya Kinjyo², Shunsaku Yasumura¹, Takashi Toyao², Daiju Matsumura³, Hiroyuki Saito⁴, Ken-ichi Shimizu¹, Norikazu Namiki², Zen Maeno²

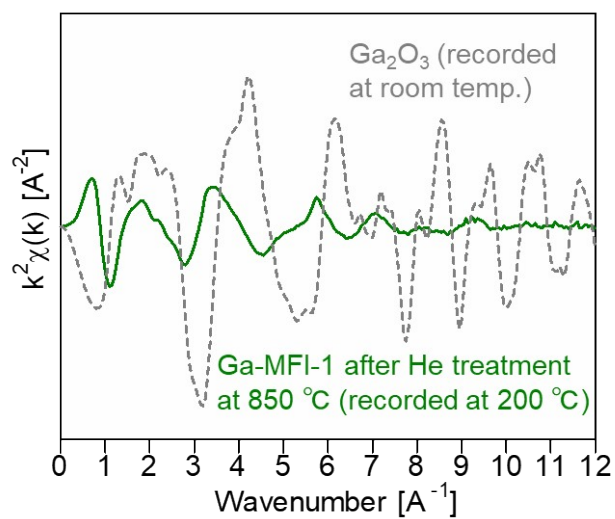


Figure S1. k^2 -Weighted EXAFS oscillations of Ga-MFI-1 after He treatment (recorded at 200 °C) and Ga_2O_3 (recorded at room temperature).

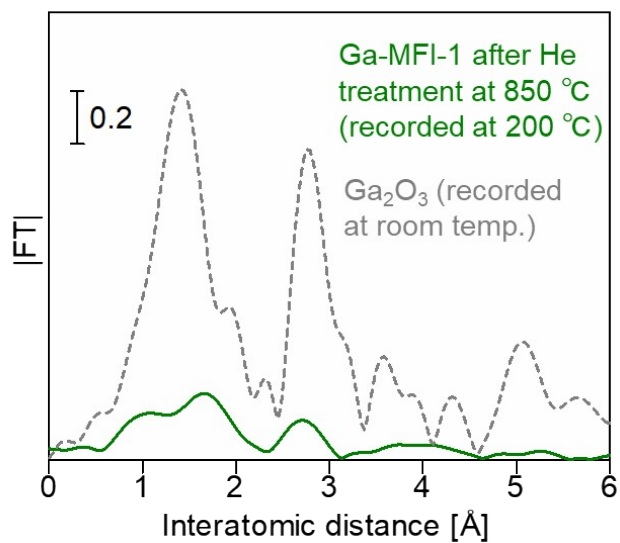


Figure S2. FT-EXAFS spectra of Ga-MFI-1 after He treatment (recorded at 200 °C) and Ga_2O_3 (recorded at room temperature). The spectra were not corrected for phase shift.

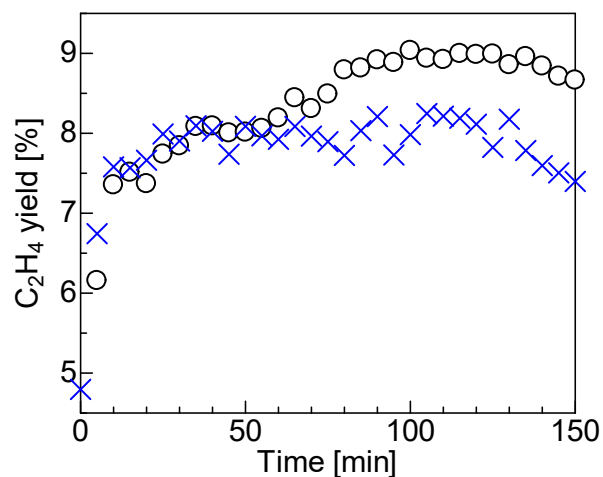


Figure S3. Comparison of time course of C_2H_4 yield in EDH over CO-treated Ga-MFI-1 (black) and Ar-treated Ga-MFI-1 (blue) at 600 °C. For CO-treated Ga-MFI-1, the oxidized Ga-MFI-1 was pretreated with 10% CO/Ar at 700 °C and then used for the EDH reaction. For Ar-treated Ga-MFI-1, the fresh Ga-MFI-1 prepared by RSSIE under H_2 flow was treated with Ar at 800 °C and then used for the reaction.

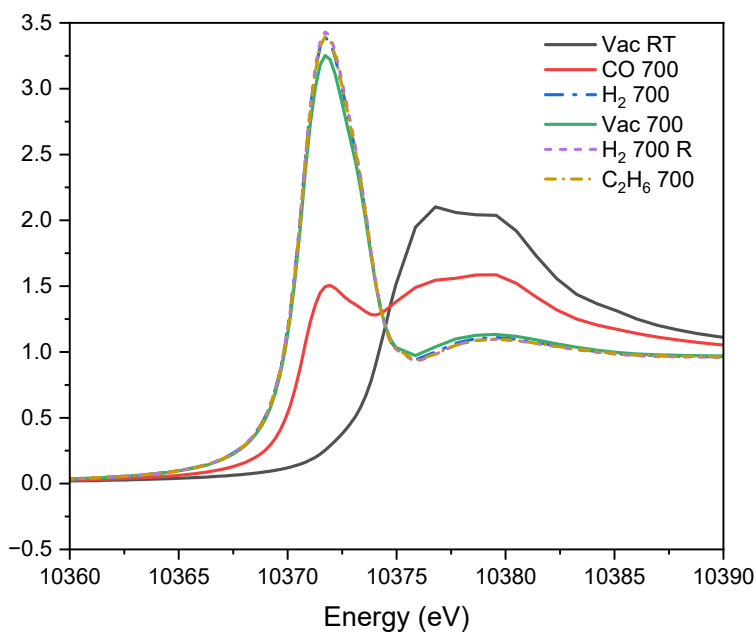


Figure S4. *In situ* Ga K-edge XAS spectra of Ga-MOR-1 obtained under various conditions including CO atmosphere. All the spectra were obtained at 700 °C, except for the first spectrum (black) was taken under room temperature.

Table S1. ΔAb_{\max} , relative amount of Ga-hydrides, and steady-state activity for Ga-exchanged zeolites with different-type frameworks

Sample	Ab_{\max} in vacuum ^[a]	Ab_{\max} in C_2H_6 ^[a]	ΔAb_{\max} ^[b]	Negative IR intensity ^[c] (index of relative amount of Ga-hydrides)	C_2H_4 yield ^[d] (index of steady-state activity)
Ga-MFI-1	2.76	3.21	0.45	0.059	38.2%
Ga-MOR-1	3.25	3.40	0.15	0.014	19.0%
Ga-CHA-1	3.10	3.21	0.11	0.003	11.2%

[a] Obtained from in situ Ga K-edge XANES spectra (recorded at 700 °C). [b] Calculated by subtraction of Ab_{\max} in vacuum from that in C_2H_6 . [c] The negative intensity at 2050 cm^{-1} in IR spectra (recorded at 50 °C) after H-D exchange reaction of H_2 -treated Ga-exchanged zeolites under D_2 flow at 200 °C (ref 26). [d] C_2H_4 yield after 3 h in nonoxidative ethane dehydrogenation using H_2 -treated Ga-exchanged zeolites at 660 °C (ref 26).