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Program Title (English) : In-situ XAFS study of highly active GaPtB catalysts under propane dehydrogenation conditions

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1. Summary

In our previous work, we successfully developed a four-component GaPtBZr/Al_2O_3 catalyst for PDH reaction using an ML model combined with a metaheuristic optimization algorithm (currently under revision). These experiments confirmed the synergistic effect of elements Ga, Pt, B, and Zr. Despite the excellent performance observed, the analysis of four-component catalysts poses significant challenges when attempting to determine the cause using conventional lab-scale analysis. Therefore, in-situ XAFS measurement techniques are an excellent probe to examine the electronic behavior and interaction between each element of catalysts containing Ga, Pt, and B (excluding Zr, which has a minor effect among the four elements).

2. Experimental

Figure 1 shows the *in-situ* XAFS experimental process of the GaPtB-*x* catalysts under pretreatment conditions. The objective of this beamtime is to investigate variation in the oxidation state and alloy formation of the GaPtB-*x* under pretreatment conditions.

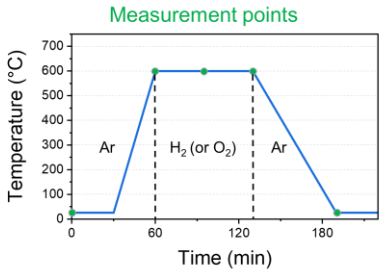

Figure 1. In-situ XAFS measurements of the GaPtB-x catalysts

3. Results and Discussion

We were performed the in-situ XAFS measurements of Ga and Pt catalysts supported on the Al_2O_3 at Pt L_3 and Ga K edges in oxidation and reduction conditions at 600 °C. The Pt and Ga formed an alloy under reduction conditions, while the excess Ga retained nanoparticles in the form of GaO_x. Under oxidation conditions, Ga and Pt were present as nanoparticles, respectively, forming multi-active species for PDH. The introduction of B increased the amount of metallic state Pt, which exhibits high PDH performance.

4. Others

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