Supporting Information

Crystal structure and microstructure changes of molybdenum nitrides traced during catalytic reaction by in situ X-ray diffraction studies.

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![Diffraction Pattern](https://example.com/diffraction_pattern.png)

- **Fig. S1:** ex situ diffraction pattern collected after ammonolysis at 800°C, Rietveld refinement plots based on different symmetries and stoichiometries.

- Fm3m Mo:N = 1:1
  - R_{wp}: 9.1
  - a: 4.2418(10) Å

- Fm3m Mo:N = 2:1
  - R_{wp}: 10.5
  - a: 4.2404(11) Å

- Pm3m Mo_{3.2}N_{2.7}
  - R_{wp}: 4.9
  - a: 4.2415(9) Å

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Fig. S2: in situ diffraction pattern collected during ammonia decomposition at 650°C after the 5th ammonia decomposition cycle using MoN-650 as catalyst.

Fm3m Mo$_2$N$_{1.7}$

$R_{wp}: 4.6$

$a: 4.1806(1)$ Å

Fig. S3: in situ diffraction pattern collected during ammonia decomposition at 650°C after the 5th ammonia decomposition cycle using MoN-8000 as catalyst.

Fm3m Mo$_2$N$_{1.6}$

$R_{wp}: 4.6$

$a: 4.1805(2)$ Å