

## Electronic Supplementary Information

### **CO<sub>x</sub>-free hydrogen production via ammonia decomposition over molybdenum nitride-based catalysts**

Atthapon Srifa, Kaname Okura, Takeou Okanishi, Hiroki Muroyama, Toshiaki Matsui, and  
Koichi Eguchi\*

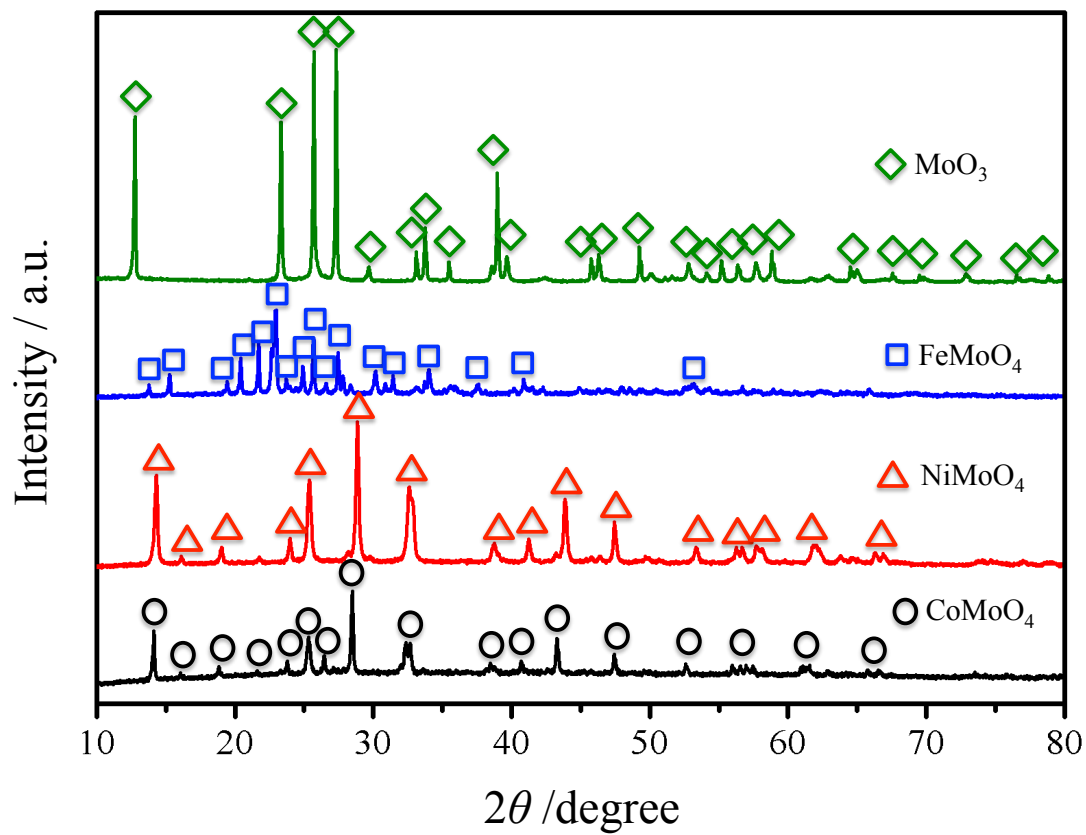
*Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto  
University, Nishikyo-ku, Kyoto 615-8510, Japan*

Correspondence should be addressed to

Koichi Eguchi

Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto  
University, Nishikyo-ku, Kyoto 615-8510, JAPAN

TEL: +81-75-383-2519, FAX: +81-75-383-2520 E-mail: [eguchi@scl.kyoto-u.ac.jp](mailto:eguchi@scl.kyoto-u.ac.jp)



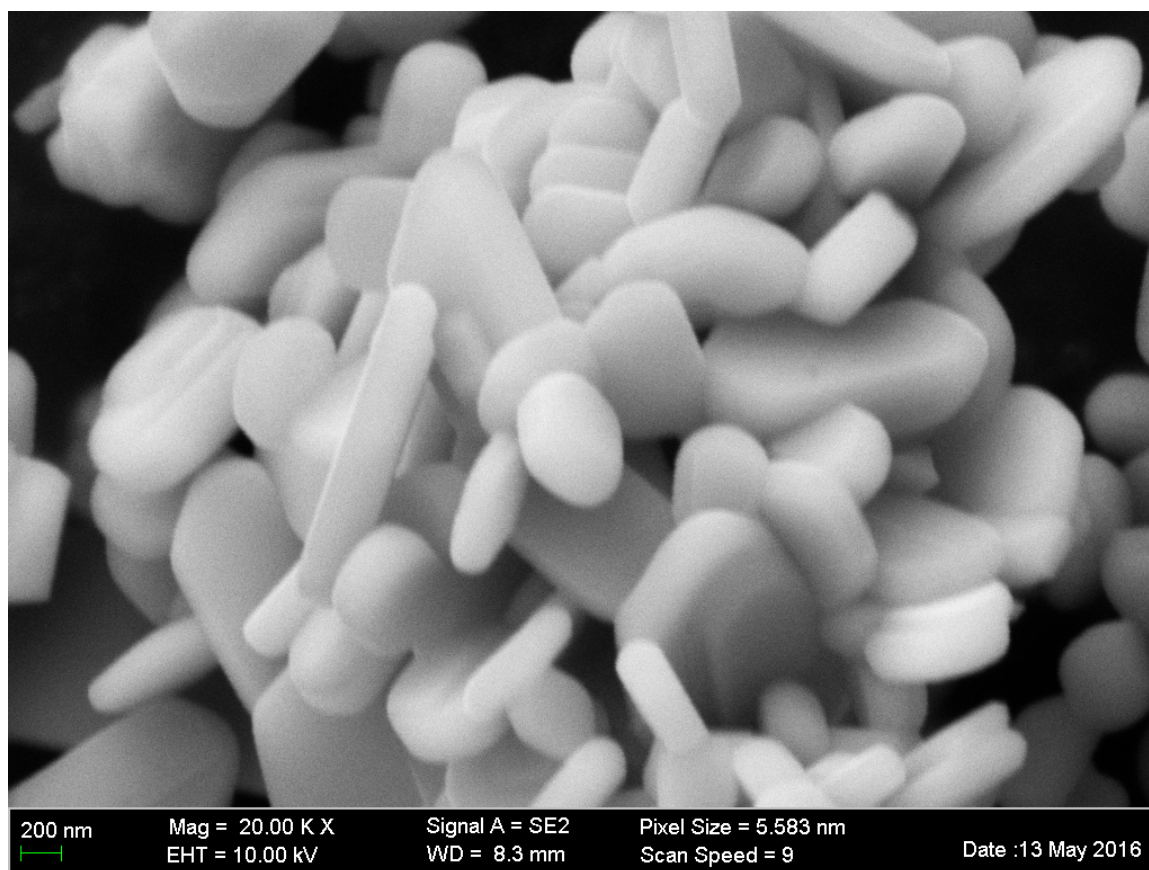
**Fig. S1** XRD patterns of the synthesized CoMoO<sub>4</sub>, NiMoO<sub>4</sub>, FeMoO<sub>4</sub> and MoO<sub>3</sub>

**Table S1** BET surface area and pore volume of the MoO<sub>3</sub>, CoMoO<sub>4</sub>, NiMoO<sub>4</sub>, and FeMoO<sub>4</sub>

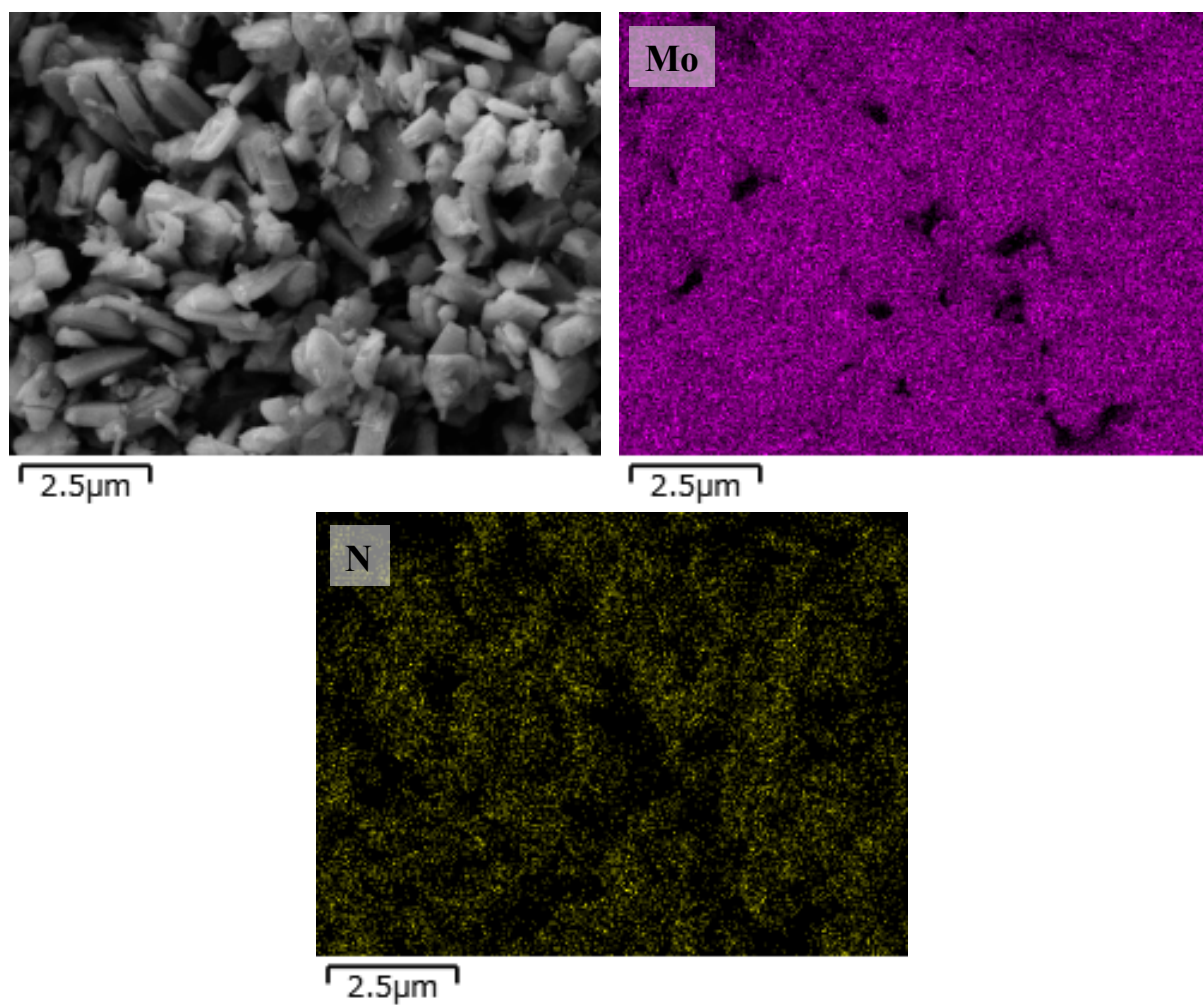
| Catalyst           | BET surface area <sup>a</sup><br>(m <sup>2</sup> g <sup>-1</sup> ) | Total pore volume <sup>b</sup><br>(cm <sup>3</sup> g <sup>-1</sup> ) |
|--------------------|--|--|
| MoO <sub>3</sub>   | 0.7  | 0.0011   |
| CoMoO <sub>4</sub> | 15.1   | 0.0087   |
| NiMoO <sub>4</sub> | 14.6   | 0.0074   |
| FeMoO <sub>4</sub> | 6.3  | 0.0042   |

<sup>a</sup> BET surface area calculated from the adsorption branch of the N<sub>2</sub> isotherm

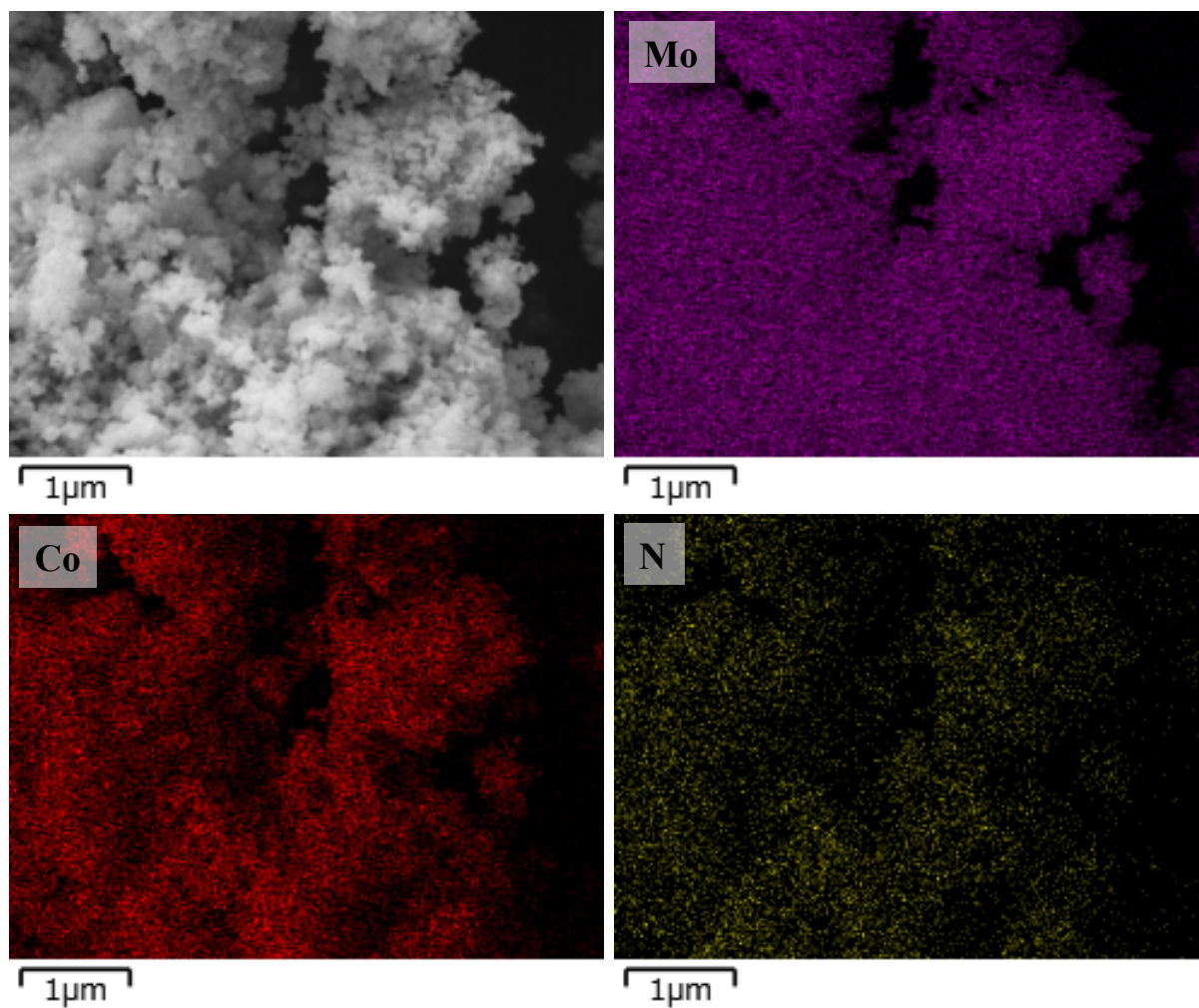
<sup>b</sup> Total pore volumes calculated from the N<sub>2</sub> adsorption at a relative pressure of 0.98



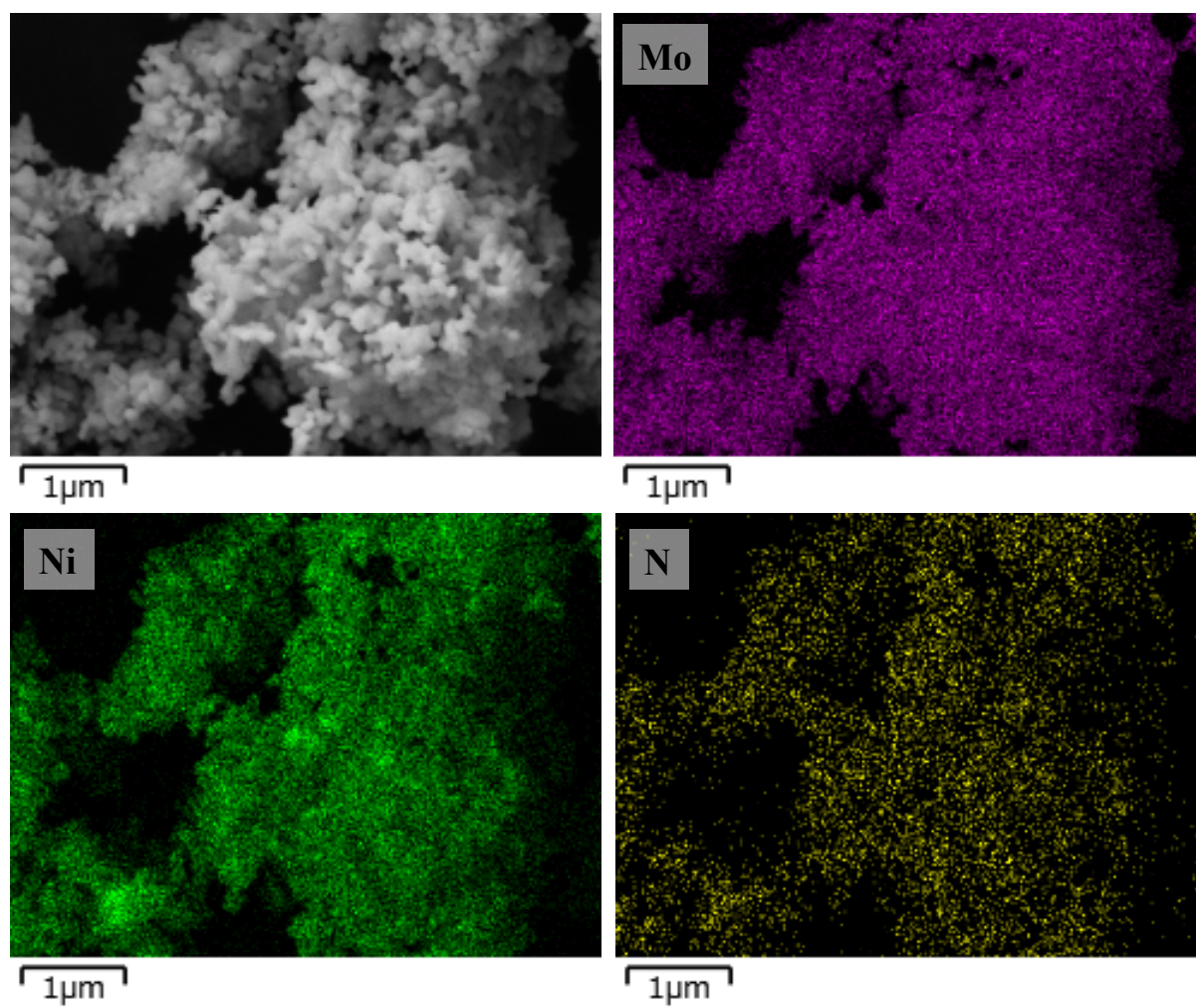
**Fig. S2** SEM image of the MoO<sub>3</sub>



**Fig. S3** SEM image and EDS mapping of the  $\text{Mo}_2\text{N}$  catalyst

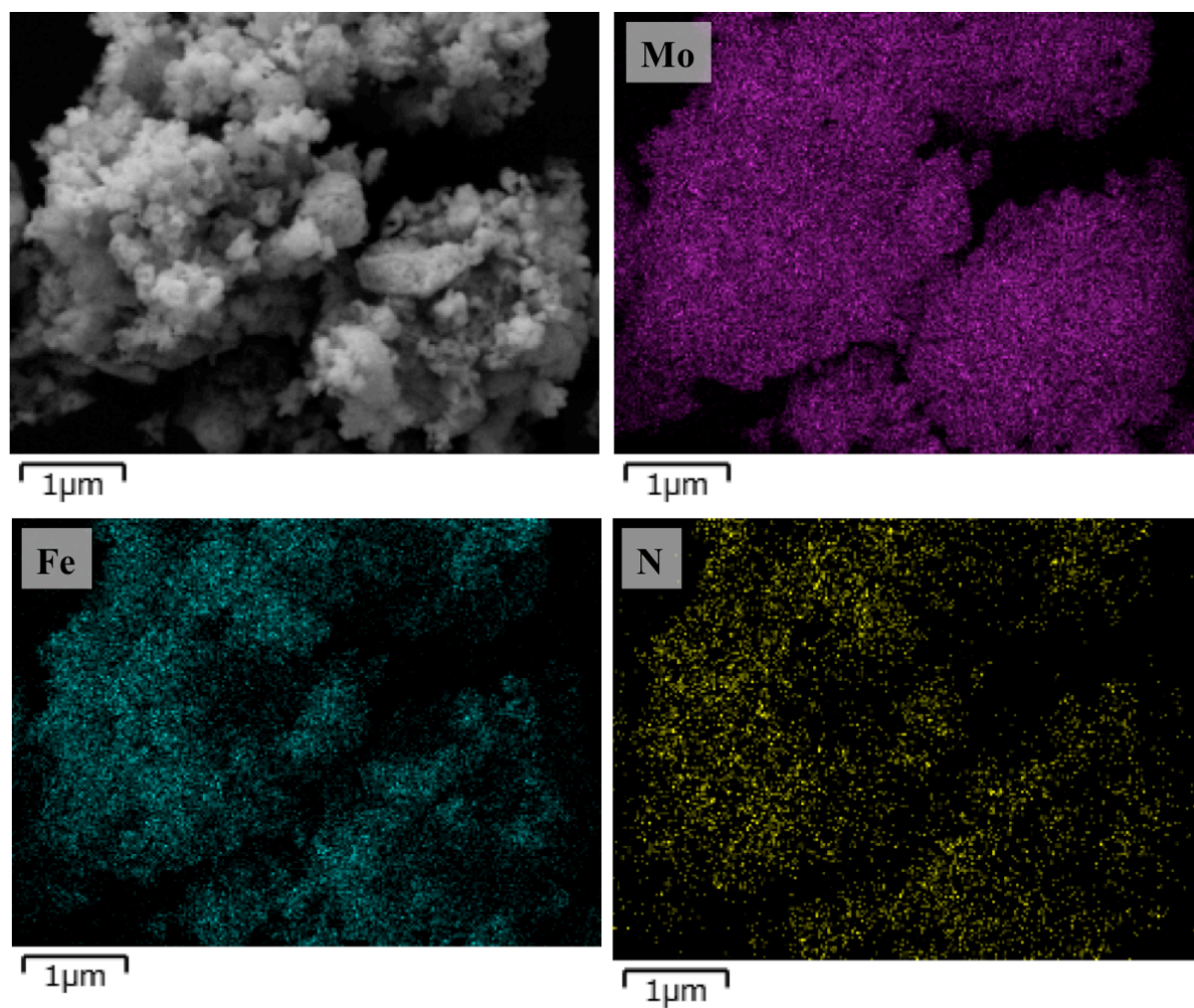


**Fig. S4** SEM image and EDS mapping of the Co<sub>3</sub>Mo<sub>3</sub>N catalyst



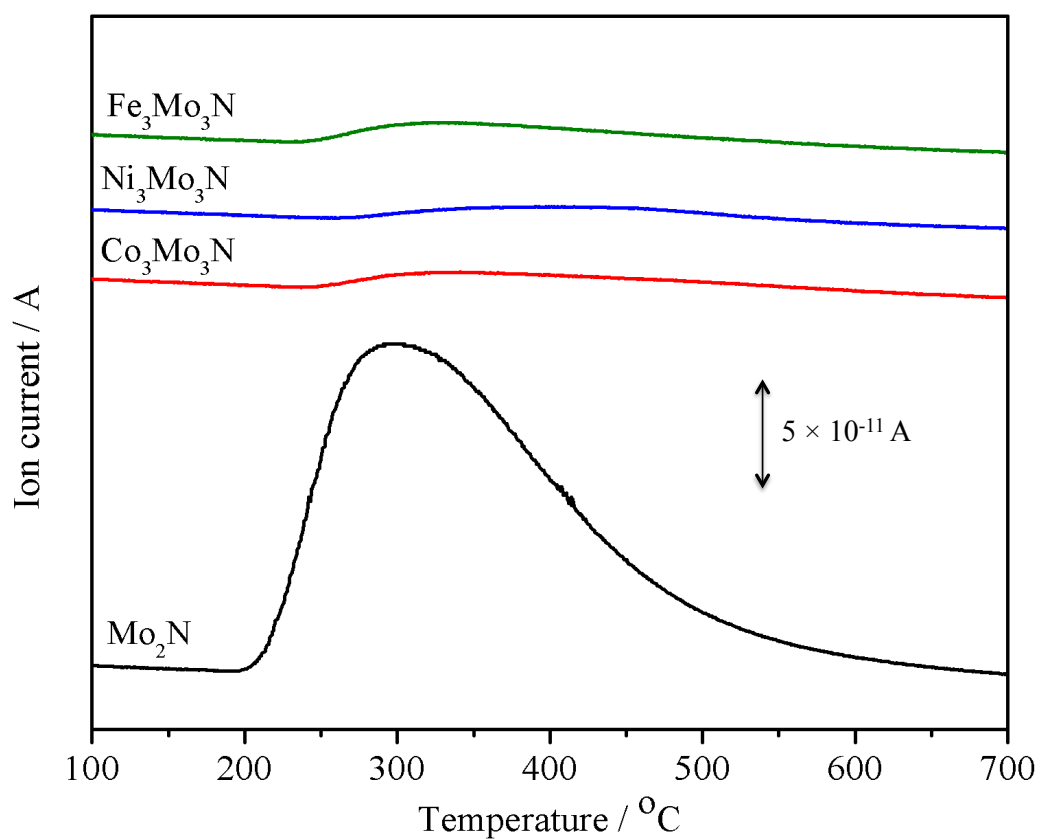
**Fig. S5** SEM image and EDS mapping of  $\text{Ni}_3\text{Mo}_3\text{N}$  catalyst



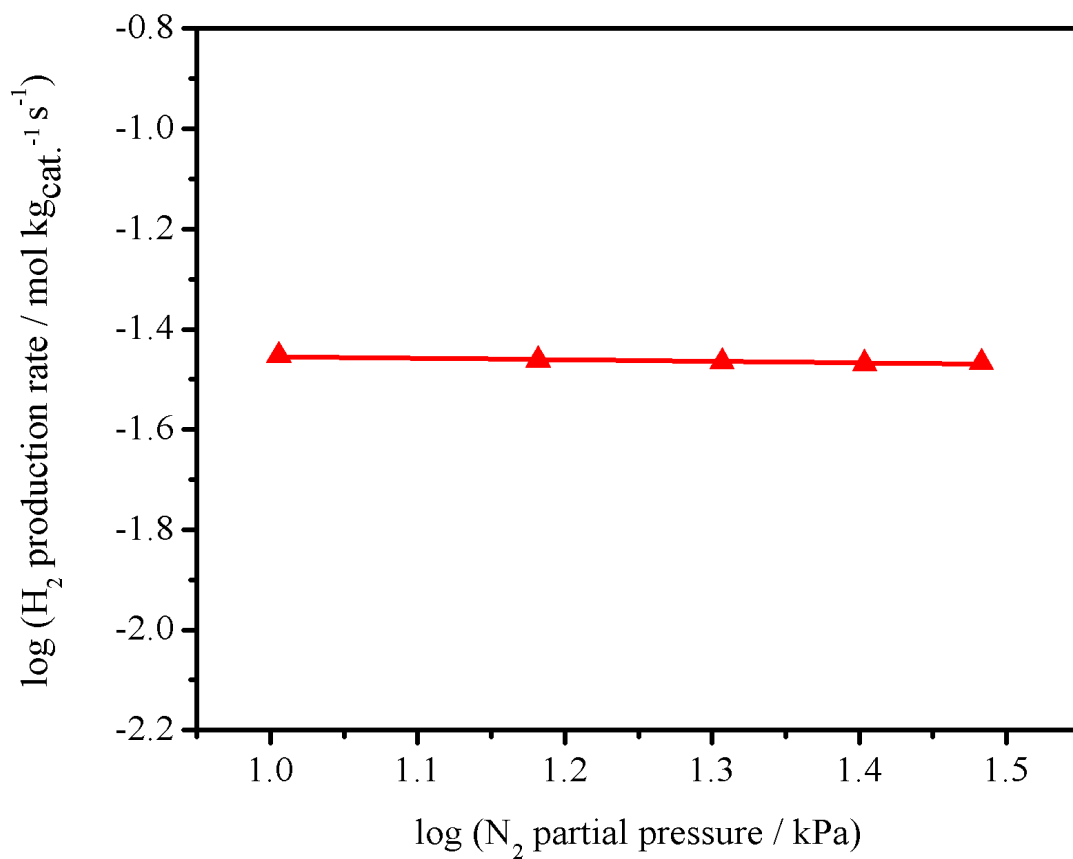


**Fig. S6** SEM image and EDS mapping of the Fe<sub>3</sub>Mo<sub>3</sub>N catalyst





**Fig. S7** Ammonia temperature-programmed desorption profiles of  $\text{Mo}_2\text{N}$ ,  $\text{Co}_3\text{Mo}_3\text{N}$ ,  $\text{Ni}_3\text{Mo}_3\text{N}$ , and  $\text{Fe}_3\text{Mo}_3\text{N}$  catalysts.



**Fig. S8** Reaction orders of N<sub>2</sub> over the Co<sub>3</sub>Mo<sub>3</sub>N catalyst at 500 °C. The partial pressure of N<sub>2</sub> was varied from 10-30 vol.% at a constant space velocity of 10,000 l kg<sup>-1</sup> h<sup>-1</sup>.