

**Switching On/Off molybdenum nitride catalytic activity in ammonia synthesis through
modulating metal support interaction**

Amanda Sfeir¹, Camila A. Teles¹, Maya Marinova², Herve Vezin³, Jean-Philippe Dacquin¹,
Axel Löfberg¹, Said Laassiri^{4*}, Sébastien Royer^{1*}

¹ Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181 – UCCS – Unité de Catalyse et Chimie du Solide, F-59000 Lille, France.

² Université de Lille, CNRS, INRA, Centrale Lille, Université Artois, FR 2638 – IMEC – Institut Michel-Eugène Chevreul, 59000 Lille, France.

³ Laboratoire de Spectroscopie pour Les Interactions La Réactivité et L'Environnement Université de Lille, UMR CNRS 8516-LASIRE, 59000 Lille, France

⁴ Chemical & Biochemical Sciences, Green Process Engineering (CBS), Mohamed VI Polytechnic University, UM6P, 43150, Benguerir, Morocco

* Corresponding authors: said.laassiri@um6p.ma, sebastien.royer@univ-lille.fr

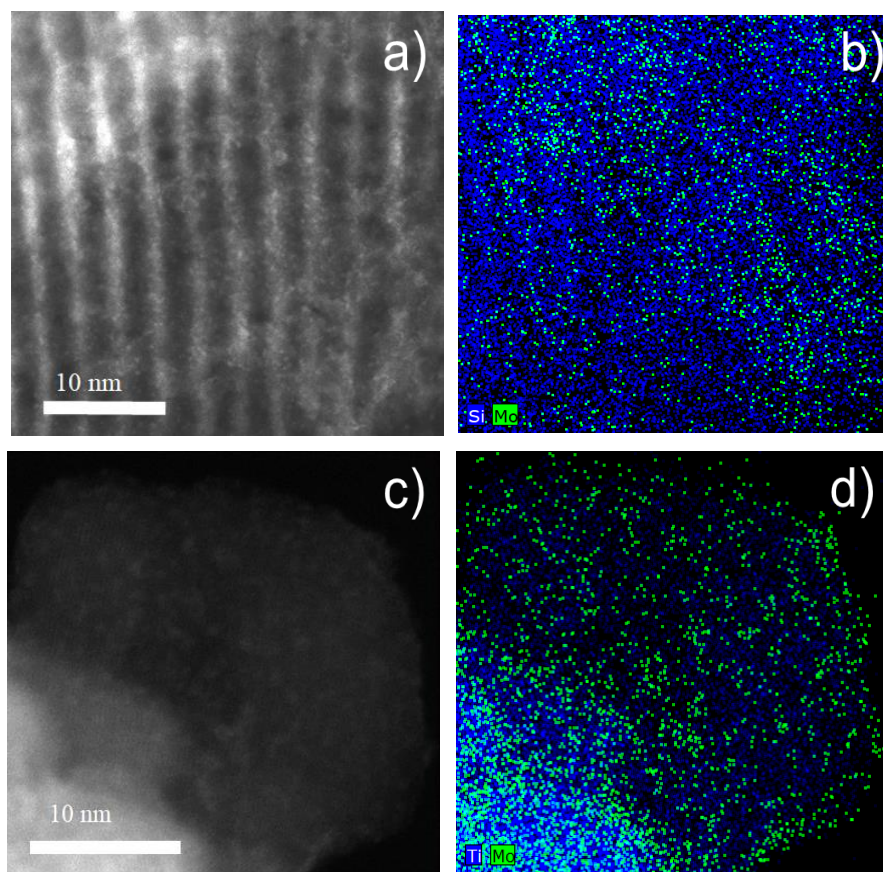


Fig. S1 Representative lower magnification HAADF images and the corresponding STEM-EDX elemental maps for 10-Mo-N/SBA-15 (a, and b) 10-Mo-N/TiO₂ (c and d)

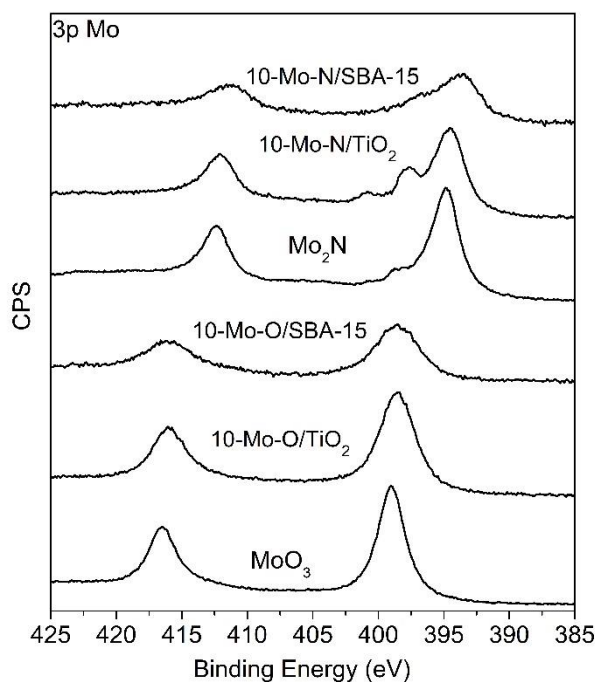


Fig. S2 XPS spectra recorded on the calcined materials in Mo 3p Region (10-Mo-O/SBA-15 and 10-Mo-O/TiO₂) and after nitridation under reaction conditions at 700°C for 2h in environmental XPS chamber

Table S1. Position of Si 2p peaks of unsupported and supported Mo based catalyst at different reactive condition

	Si 2p peak position		Surface composition	
	Si-O-Si	Si-O-H	Si-O-Si (%)	Si-O-H (%)
10-Mo/SBA-15	104.00	103.16	54.96	45.04
10-Mo-N/SBA-15*	104.00	103.05	29.58	70.42

* catalyst subject to pre-treatment under reaction condition at 700°C for 2h in environmental XPS chamber before analysis

Table S2. Position of Ti 2p peaks of unsupported and supported Mo based catalyst at different reactive condition

	Ti 2p peak position	
	Ti 2p _{3/2}	Ti 2p _{1/2}
10-Mo/TiO₂	458.89	464.61
10-Mo-N/TiO₂*	459.51	465.23

* catalyst subject to pre-treatment under reaction condition at 700°C for 2h in environmental XPS chamber before analysis

Table S3. Atomic Concentration of Mo on the surface before and after nitridation according to XPS.

% atm Concentration of Mo	Oxide	Nitride
10-Mo/TiO ₂	12.5	9.86
10-Mo/SBA-15	4.3	3.57

Table S4. H₂ uptake from TPR on MoO₃ 10-Mo-O/TiO₂ and 10-Mo-O/SBA-15

Sample	H ₂ uptake (mmol g ⁻¹)	
	Exp. ^f	Calc. ^g
MoO ₃	23.3	20.8
10-Mo-O/SBA-15	1.9	2.2
10-Mo-O/TiO ₂	2.9	2.8

Fig. S3 H₂-TPR profiles of TiO₂ and SBA-15

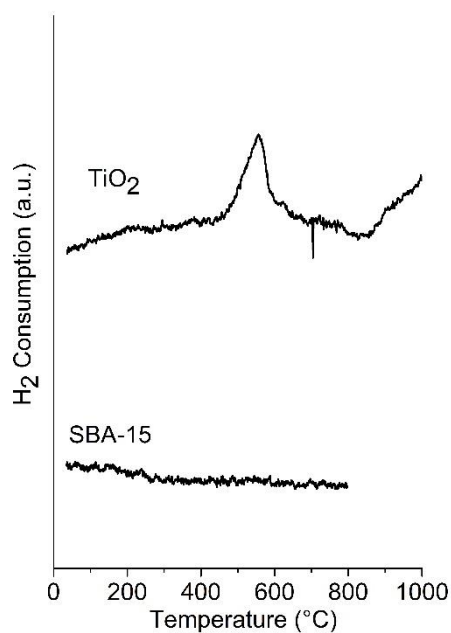


Table S5. H₂ desorption quantities for H₂-TPD in the range 25 – 550 °C

Catalyst	H ₂ desorption (mmol/g)
10-Mo-N/TiO ₂	0.11481
10-Mo-N/SBA-15	0.13033