## **Electronic Supplementary Information**

## N-doped Carbon Encapsulated Molybdenum Carbide as Efficient Catalyst for

## **Oxidant-Free Dehydrogenation of Alcohols**

Yan Leng\*, Jingjing Li, Chenjun Zhang, Pingping Jiang, Yue Li, Yuchen Jiang, Shengyu Du

The Key Laboratory of Synthetic and Biological Colloids, Ministry of Education, School of Chemical and Material Engineering, Jiangnan University, Wuxi 214122, Jiangsu, China. Email: <a href="mailto:yanleng@jiangnan.edu.cn">yanleng@jiangnan.edu.cn</a>



Figure S1. <sup>1</sup>H NMR spectrum of DIM.



Figure S2. XRD patterns of PMo@DIM<sub>400/800</sub>



Figure S3. Raman patterns of PMo@DIM<sub>400/800</sub>



Figure S4. (A) SEM and (B) TEM images of PMo@DIM-AN.



Figure S5. EDS elemental mapping images of Mo, P, C, N, O elementals on PMo@DIM- $AN_{400/800}$ .



Figure S6. The energy dispersive X-ray (EDX) spectra of PMo@DIM-AN<sub>400/800</sub>.



Figure S7. XPS survey spectrum of (a) PMo@DIM-AN<sub>400/800</sub>, (b) PMo@DIM-AN<sub>800</sub>, (c) PMo@DIM<sub>400/800</sub>.



Figure S8. GC spectrum for oxidant-free dehydrogenation of benzyl alcohol over PMo@DIM- $AN_{400/800}$ .



Figure S9. The influence of catalyst amount, reaction time, and reaction temperature on the oxidant-free dehydrogenation of benzyl alcohol over PMo@DIM-AN<sub>400/800</sub>.



**Figure S10**. (A) Catalytic reusability of PMo@DIM-AN<sub>400/800</sub> for dehydrogenation of benzyl alcohol: (B) XRD patterns of (a) fresh PMo@DIM-AN<sub>400/800</sub>, (b) recycled from dehydrogenation of benzyl alcohol. (C) TEM and (D) SEM images of recovered PMo@DIM-AN400/800.

		OH Catalyst		+ H <sub>2</sub>	
Entry	solvent	Temperature	Time (h)	Yield <sup>a</sup> (%)	Sel <sup>b</sup> (%)
		(°C)			
1	CH <sub>3</sub> CN	90	6	8.1	100
2	methylbenzene	110	6	21.2	100
3	DMF	120	6	32.0	100
4	DMF	130	8	37.6	100
5	DMSO	120	4	100	100
6	H <sub>2</sub> O	110	8	24.3	100
7	1,4-dioxane	110	8	23.2	100
8	Solvent free	120	8	24.7	100
9	Solvent free	130	8	27.0	100

Table S1. Catalytic performances of PMo@DIM-AN $_{400/800}$  for dehydrogenation of benzyl alcohol in various solvents.

Reaction conditions: benzyl alcohol (2 mmol), solvent (4 mL), catalyst (0.05 g), <sup>a</sup> Yield of the substrate determined by GC, <sup>b</sup> Selectivity for the benzaldehyde product.