Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Bimetallic molybdenum nitride Co_3Mo_3N: A new promising catalyst for CO_2 reforming of methane

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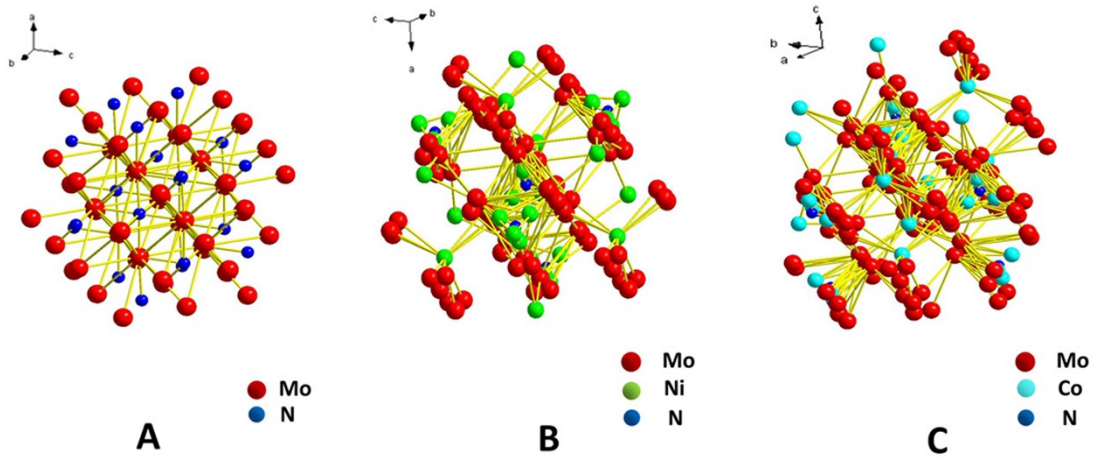

Fig. S1 Schematic diagrams of crystal structure of catalysts: A, Mo_2N; B, Ni_3Mo_3N; C, Co_3Mo_3N.

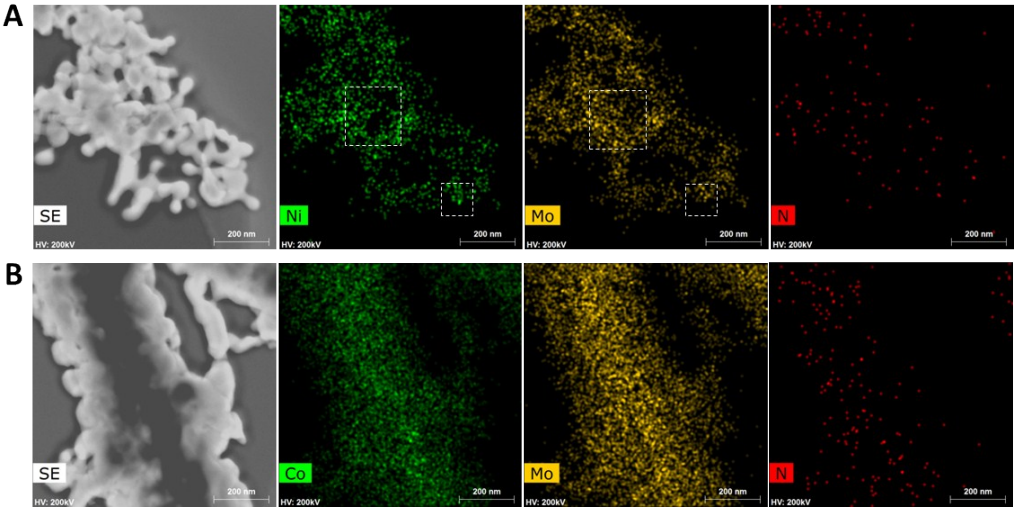

Fig. S2 STEM-mapping images of catalysts: A:Ni_3Mo_3N, B: Co_3Mo_3N.

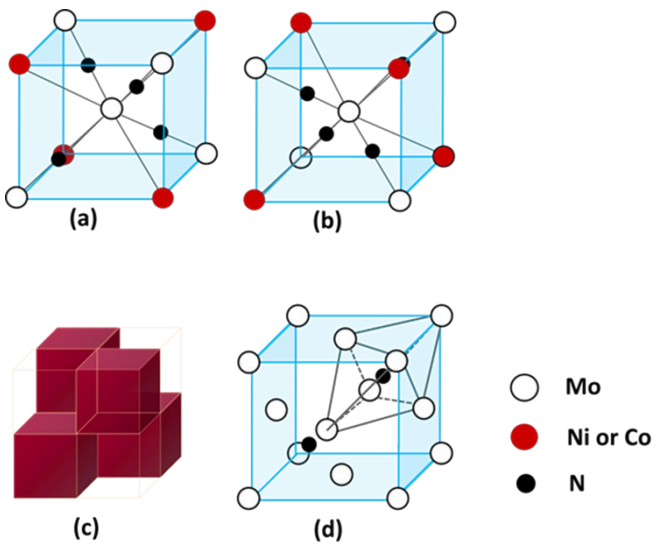

Fig. S3 Schematic representation of the catalysts structure. (a) and (b): typical Ni_3Mo_3N or Co_3Mo_3N unit cell; (c): the sub-cells of Ni_3Mo_3N or Co_3Mo_3N (d): crystallographic structure of Mo_2N.

Although Ni_3Mo_3N or Co_3Mo_3N exhibits a large bcc unit cell (a and b), its structure can be visualized as composed of two sub-cells, alternately stacked inside a cubic array (c); In (c), the sub-cells assume a diamond cubic-type of arrangement in which the Ni/Co and Mo atoms are located at the corners and center of the cubic cells.

Table S1 Summarization of the activity of catalysts for dry reforming of methane

	Catalysts	Reaction condition				Conversion (%)		Reaction rate[a] (mol/g·s)		Ref.
		T (°C)	Pressure	Atmosphere	Time (h)	CH_4	CO_2	CH_4	CO_2	
1	Co_3Mo_3N	800	Atmospheric pressure	CH_4/CO_2 = 1:1 GHSV = 6,000 ml/g_{cat}·h	50	91	96	3.16×10^{-7}	3.26×10^{-7}	this work
2	$Ni/CeAlO_3$-Al_2O_3	800	Atmospheric pressure	CH_4 : CO_2=1:1, GHSV=20,000ml/g·min	250	80	90	9.07×10^{-7}	1.02×10^{-6}	45
3	Ni/SiO_2	800	Atmospheric pressure	CO_2:CH_4:N_2=1:1:1 GHSV=36,000ml/g_{cat}·h	90	60	73	2.57×10^{-6}	3.12×10^{-6}	46
4	Ni/MgO-ZrO_2	750	Atmospheric pressure	CH_4:CO_2:O_2 = 1.5:1:0.25	6.6	62	69	1.24×10^{-6}	9.12×10^{-7}	47
5	$Ni/MgAl_2O_4$	750	P = 1 atm	CH_4:CO_2 = 1:1 GHSV = 50,000 ml/g_{cat}·h	55	83	93	7.80×10^{-7}	8.70×10^{-7}	48
6	Ni−1Ce−Al	700	Atmospheric pressure	CH_4:CO_2=1:1, GHSV=36,000 L/h·g_{cat}	80	70	-	1.86×10^{-5}	-	39
7	TiO_2-Ni	800	Atmospheric pressure	CH_4:CO_2 = 1:1	60	24	42	1.26×10^{-7}	2.76×10^{-7}	49
8	Ni-Mo_2C/La_2O_3	800	Atmospheric pressure	CH_4:CO_2=1:1, F/W=12,000ml/g·h	50	62	80	3.80×10^{-6}	4.90×10^{-6}	50

9	Mo_2C	500	Atmospheric pressure	CH_4:CO_2 = 1 : 1	5	10	19	4.53×10^{-8}	8.61×10^{-8}	51
10	MoC_{1-x}(X=0.5)	500	Atmospheric pressure	CH_4:CO_2 = 1 : 1	15	58	78	2.63×10^{-7}	3.53×10^{-7}	51
11	Mo_2C/ZrO_2	500	Atmospheric pressure	CH_4:CO_2 = 1 : 1	5	13	25	5.89×10^{-8}	1.13×10^{-7}	51
12	Ni-Mo/SBA-15	800	P=1atm,	CH_4:CO_2 = 1 : 1 GHSV=4,000ml/g·h	600	94	-	2.66×10^{-7}	-	24
13	Mo_2C	850	1 bar	CH_4:CO_2=1:1, GHSV=of 3,800/h	2	62	-	5.62×10^{-9}	-	15

[a]The reaction rate values of catalysts were calculated by the equation as follows:

$$r = \frac{cXV\mathrm{P_{atm}}}{\mathrm{m_{cat}w_{metal}RT}}(mol/\mathrm{sg})$$

where r= reaction rate, c = concentration of CH_4 in the feed gas, X = conversion of CH_4, V = total flow rate, P_{atm} = atmospheric pressure, equal to 101.3 KPa, m_{cat} = mass of catalyst used for measurement, w_{metal} = active metal loading, R = molar gas constant, equal to 8.314 Pa m^3 mol^{-1} K^{-1}, T = room temperature.