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Supporting Information

Molybdenum Carbide Chemical Sensor with Ultrahigh Signal-to-Noise Ratio and Ambient Stability

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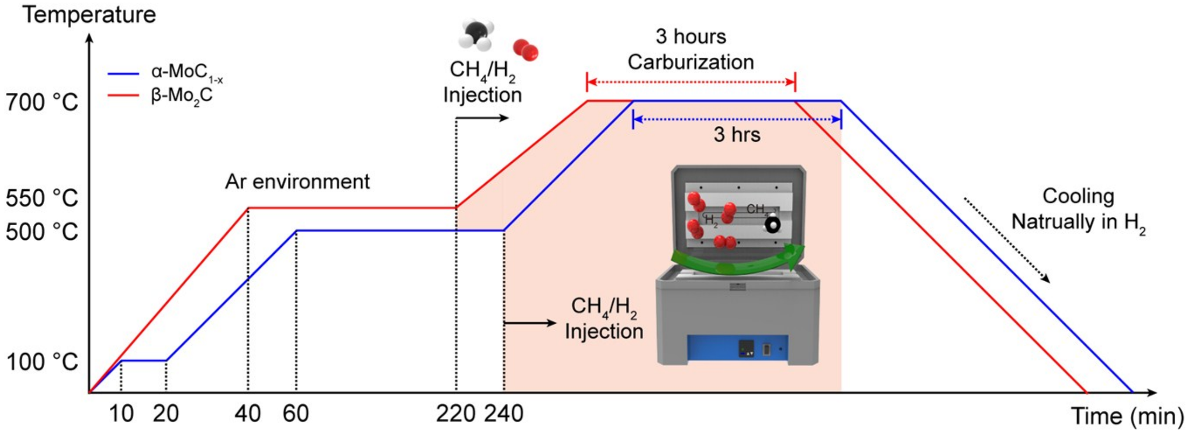

Figure S1. Schematic illustration of molybdenum carbide synthesis. x-axis represents reaction time and y-axis shows reaction temperature.

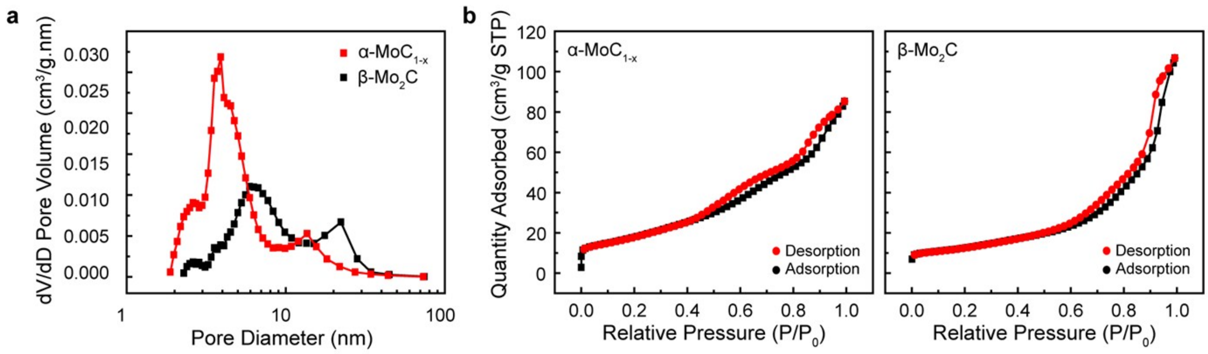

Figure S2. (a) Barrett-Joyner-Halenda (BJH) pore size distributions of synthesized molybdenum carbides (represented as differential pore volume against log scale of pore diameter). **(b)** Nitrogen adsorption isotherm linear plot by Brunauer-Emmett_Teller (BET) model for two phases of molybdenum carbides

Material	BET Surface Area (m^2/g)	Pore Volume (cm^3/g)	Average Pore Diameter (nm)
Commercial MoC_x	0.6031	0.002324	46.2534
α-MoC_{1-x}	66.0359	0.138961	6.5202
β-Mo_2C	44.0782	0.171089	11.7959

Table S1. The BET surface area, pore volume and average pore diameter information of molybdenum carbides.

HR-TEM lattice fringe analysis

1. Cubic structure (MoC_{1-x}, JCPDS 01-077-7176)

$$a = b = c = 4.244973\ \text{Å}, \qquad \alpha = \beta = \gamma = 90^0$$

$$|\vec{a}^*| = |\vec{b}^*| = |\vec{c}^*| = \frac{1}{a}$$

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{111} = \frac{4.244973\ \text{Å}}{\sqrt{3}} = 2.45\ \text{Å} \quad , \qquad d_{220} = \frac{4.244973\ \text{Å}}{\sqrt{8}} = 1.501\ \text{Å}$$

$$\cos\emptyset = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

$$\cos\emptyset = \frac{4}{\sqrt{3}\sqrt{8}} = \quad 0.8165$$

$$\therefore \emptyset = 35.26^0$$

2. Orthorhombic structure (β-Mo_2C, JCPDS 01-077-0720)

$$a \neq b \neq c, \qquad a = 6.041758\ \text{Å}, \qquad b = 4.745728\ \text{Å}, \qquad c = 5.214426\ \text{Å}$$

$$\alpha = \beta = \gamma = 90^0$$

$$|\vec{a}^*| = \frac{1}{a}\ , |\vec{b}^*| = \frac{1}{b}\ , |\vec{c}^*| = \frac{1}{c}$$

$$d_{hkl} = \frac{1}{\sqrt{(\frac{h}{a})^2 + (\frac{k}{b})^2 + (\frac{l}{c})^2}}$$

$$d_{020} = \frac{1}{\sqrt{\frac{4}{4.745728^2}}}\text{Å} = 2.37\ \text{Å}$$

$$d_{211} = \frac{1}{\sqrt{\frac{4}{6.041758^2} + \frac{1}{4.745728^2} + \frac{1}{5.214426^2}}}\text{Å} = 2.29\ \text{Å}$$

$$\cos \emptyset = \frac{\frac{h_1 h_2}{a^2} + \frac{k_1 k_2}{b^2} + \frac{l_1 l_2}{c^2}}{\sqrt{\frac{h_1^2}{a^2} + \frac{k_1^2}{b^2} + \frac{l_1^2}{c^2}}\sqrt{\frac{h_2^2}{a^2} + \frac{k_2^2}{b^2} + \frac{l_2^2}{c^2}}}$$

$$\cos \emptyset = \frac{\frac{2}{b^2}}{\sqrt{\frac{4}{b^2}}\sqrt{\frac{4}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}}} = 0.48245$$

$$\therefore \emptyset = 61.15^0$$

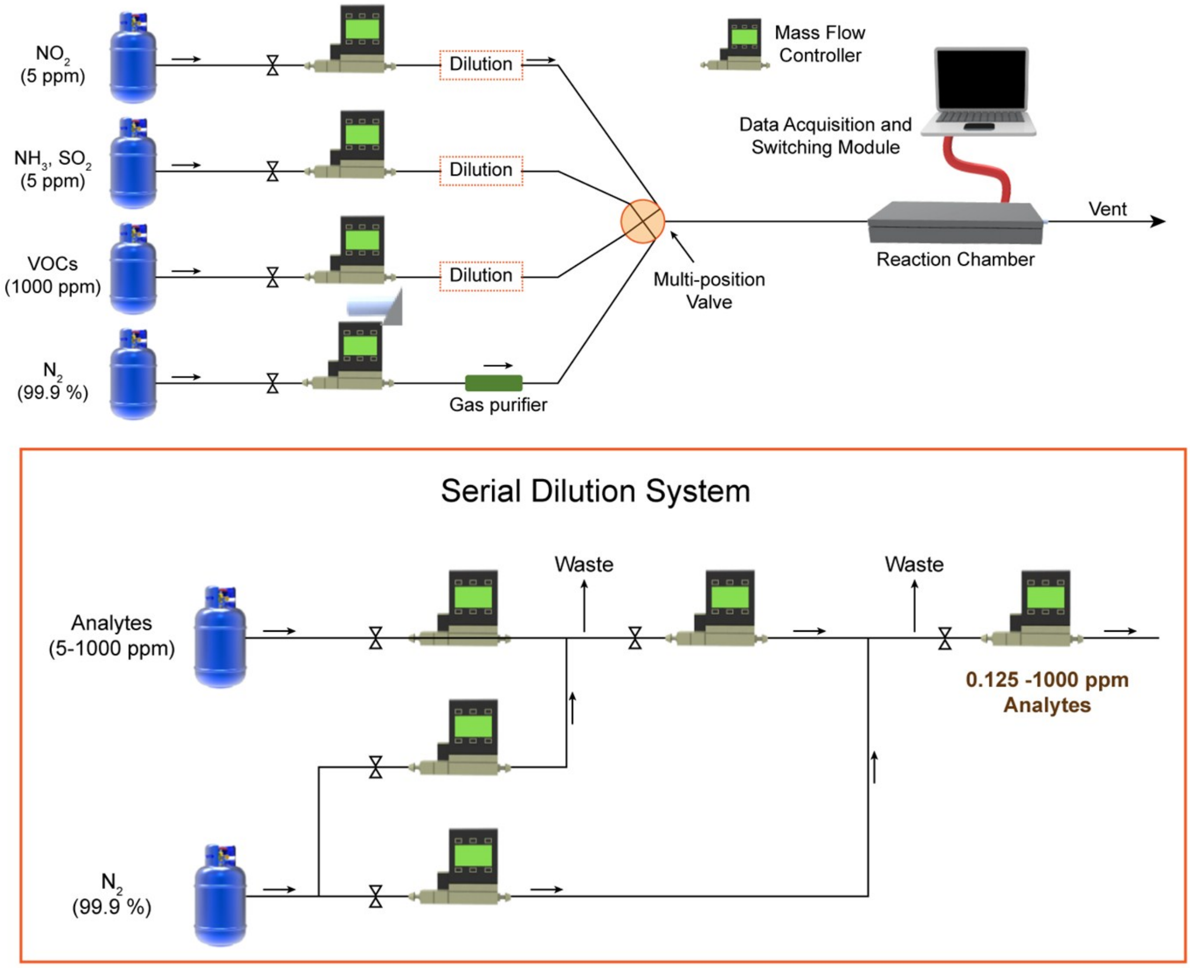

Figure S3. Schematic of the overall gas delivery system. Various analytes and N_2 was introduced in a controlled manner into the reaction chamber by using the MFC, tubing system, and multi-position valve. The serial dilution system was also used to obtain 2.5–30000 ppm concentrations of the analyzed gas.

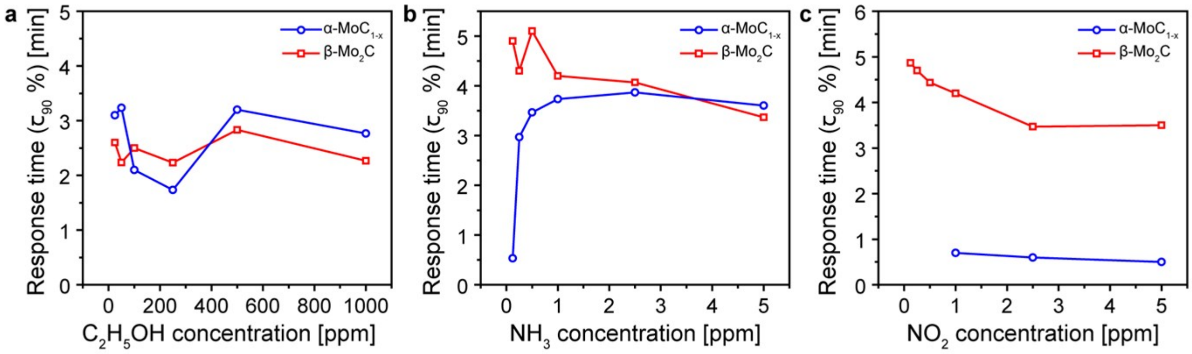

Figure S4. Response time of the α-MoC_{1-x} and β-Mo_2C sensors onto wide concentration range of **(a)** ethanol, **(b)** NH_3 and **(c)** NO_2.

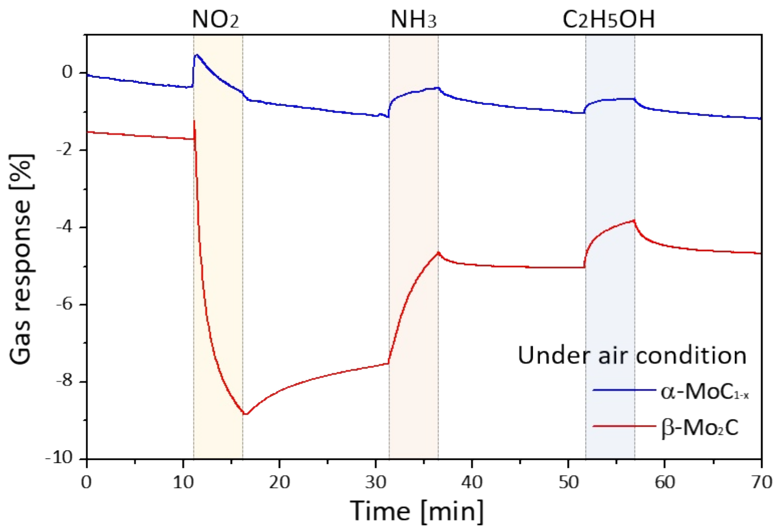

Figure S5. The real-time NO_2 (5 ppm), NH_3 (5 ppm), C_2H_5OH (1000 ppm) response behavior of the one-year old α-MoC_{1-x} and β-Mo_2C sensors under the air condition.

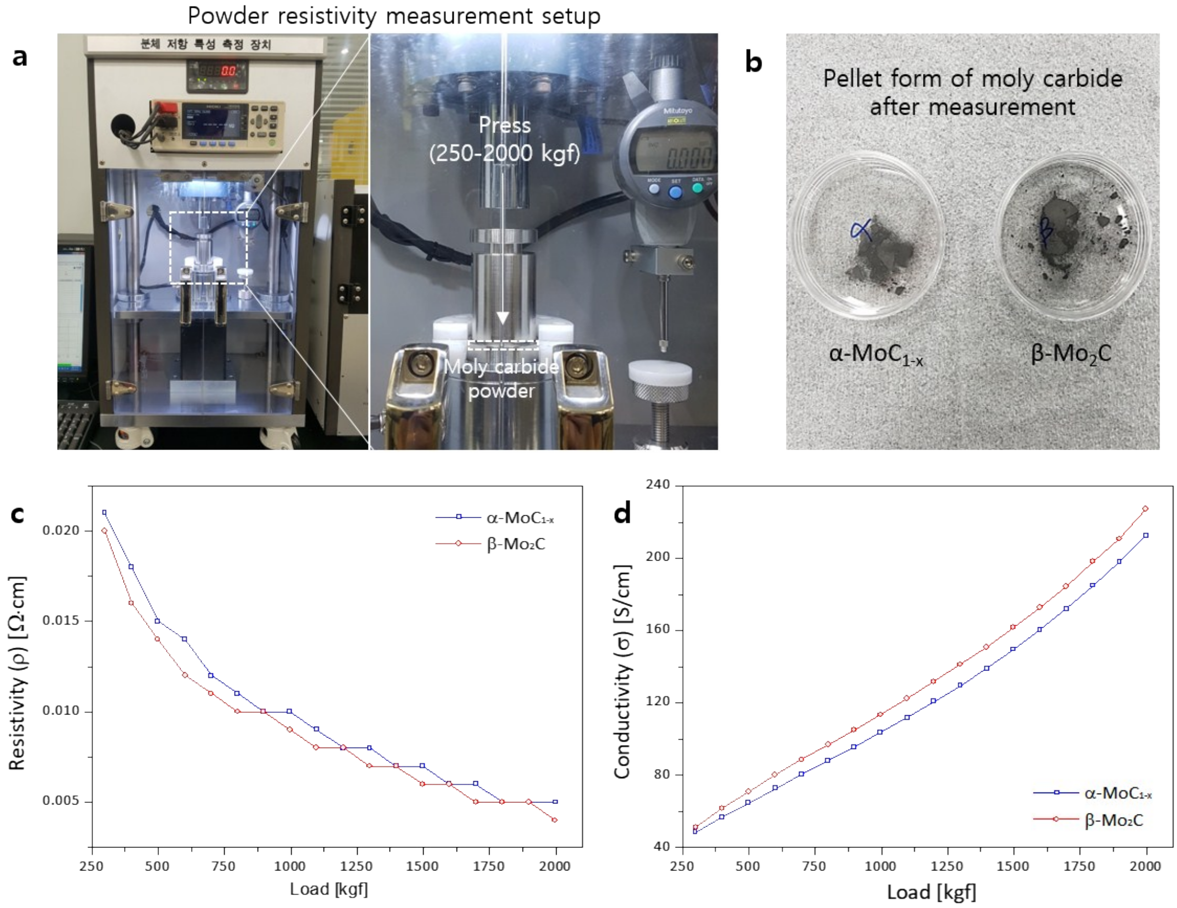

Figure S6. (a) Photo-image of the powder resistivity measurement setup (HPRM-M2, HANTECH^{TM}). (b) Pellet form of the α-MoC_{1-x} and β-Mo_2C after measurement with pressing. (c) Resistivity and (d) conductivity of the α-MoC_{1-x} and β-Mo_2C with varied pressure.