Supplementary Information

Nanorod structure tuning and defect engineering of MoO_x for high performance SERS substrates

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Table S1 Fabrication parameters of MoO_x rod-like SERS substrate

Sputtering parameter	Parameter value	Unit
Substrate temperature	30	^0C
Target-to-substrate distance	7	cm
Base pressure	$1.48x10^{-6}$	Torr
Working gas pressure	$8.35x10^{-3}$	Torr
Power	60	W
Ratio between Ar: O_2 (99.99% purity)	10:2	sccm

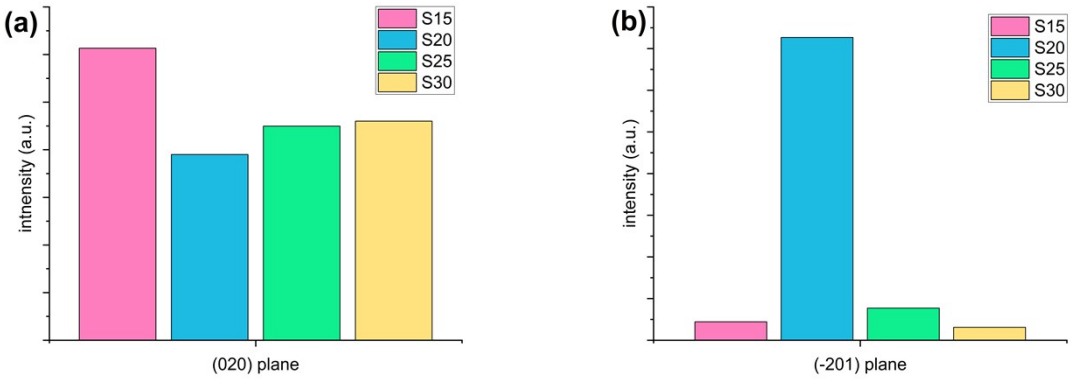

Fig S1. Comparison intensity of X-ray diffraction pattern of MoO_x thin films deposited at various sputtering time on glass substrate

a) at (020) plane for sample S15, S20, S25, and S30;

b) at (-201) plane for sample S15, S20, S25, and S30.

Table S2: Lattice parameters and crystal sizes of samples S15, S20, S25, and S30

	MoO_3 (standard value) [28]	**S15**	**S20**	**S25**	**S30**
Lattice parameter					
a (Å)	3.962	3.963	3.970	3.962	3.960
b (Å)	13.858	13.887	13.887	13.891	13.888
c (Å)	3.696	3.698	3.698	3.696	3.698
Crystal size (nm)					
(020)		71.3	77.6	86.0	96.7

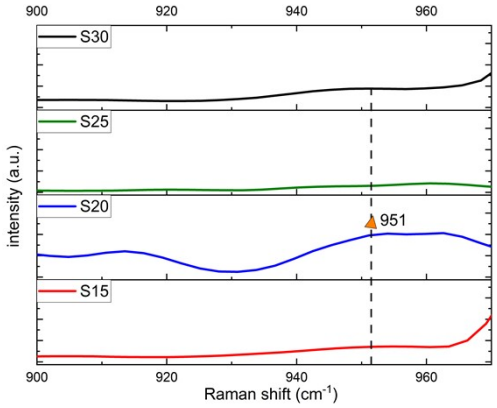

Fig. S2. Raman intensity at 951 cm^{-1} peak for S15, S20, S25, and S30 samples.

Table S3: The vibration modes and intensities of characteristic peaks in the Raman spectra for S15, S20, S25, and S30 samples.

Band frequency (cm^{-1})	**Representation**[31]	**Attribution**[31]
115	B_{2g}	Translational rigid MoO_4 chain mode along "c" direction Tc
127	B_{3g}	Translational chain mode along "c" direction (T_c)
158	A_g/B_{1g}	Translational chain mode along "b" direction (T_b)
198	B_{2g}	τ O=M=O twist
216	A_g	Rotational rigid MoO_4 chain mode R_c
245	B_{3g}	τ O=M=O twist
283	B_{2g}	δ O=M=O wagging
337	A_g, B_{1g}	δ O-M-O bend
378	B_{1g}	δ O-M-O scissor
473	A_g	υ_{as} O–M–O stretch and bend
663	B_{2g}, B_{3g}	υ_{as} O–M–O stretch
815	A_g	υ_s M=O stretch MoO_6
990	A_g, B_{1g}	υ_{as} M=O asymmetric stretch

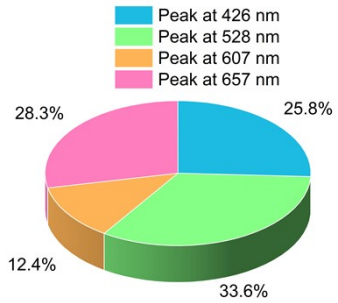

Fig. S3. The pie charts illustrate the contribution of component emissions to the total PL spectrum of S20.

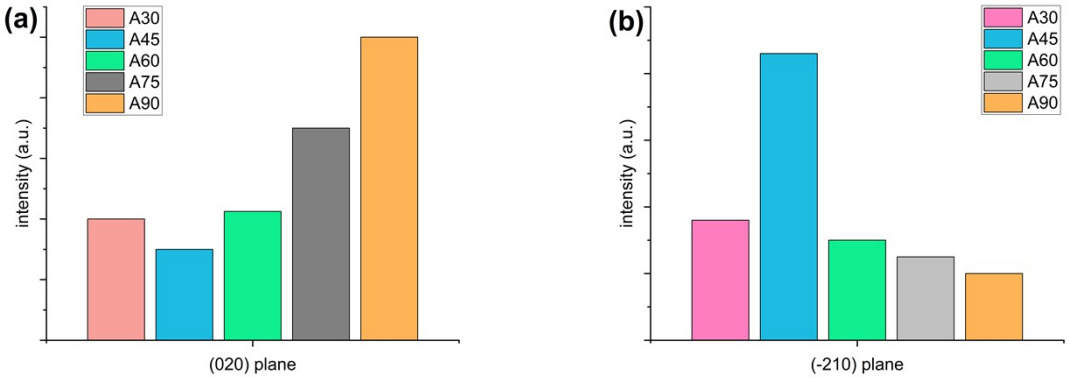

Fig. S4. Comparison intensity of X-ray diffraction pattern of MoO_x thin films deposited at various annealing time on glass substrate. a) at (020) plane for sample A30, A45, A60, A75, and A90. b) at (-201) plane for sample A30, A45, A60, A75, and A90.

Table S4: Lattice parameters and crystal sizes of samples A30, A45, A60, A75, and A90.

	MoO_3 (standard value)[28]	**A30**	**A45**	**A60**	**A75**	**A90**
Lattice parameter (Å)						
a (Å)	3.962	3.970	3.974	3.965	3.963	3.963
b (Å)	13.858	13.885	13.886	13.881	13.881	13.886
c (Å)	3.696	3.695	3.698	3.700	3.697	3.697
Crystal size (nm)						
(020)		77.5	85.5	86.0	85.5	86.0
(110)		43.4	54.1	61.9	61.9	61.9

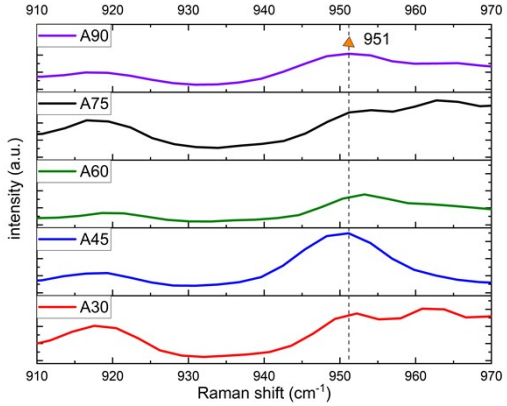

Fig. S5. Raman intensity at 951 cm^{-1} wavenumber for A30, A45, A60, A75, and A90 samples

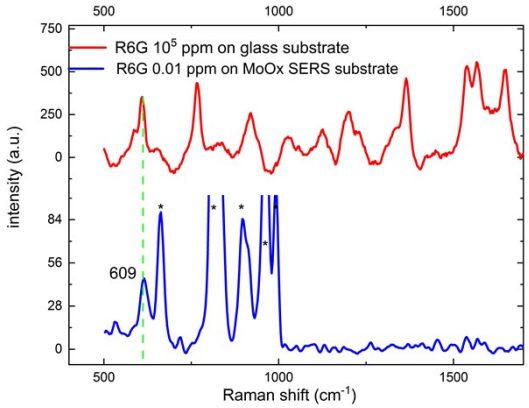

Fig. S6. Raman spectra of R6G at 10^5 ppm on glass substrate and 0.01ppm onto SERS substrate to calculate EF.

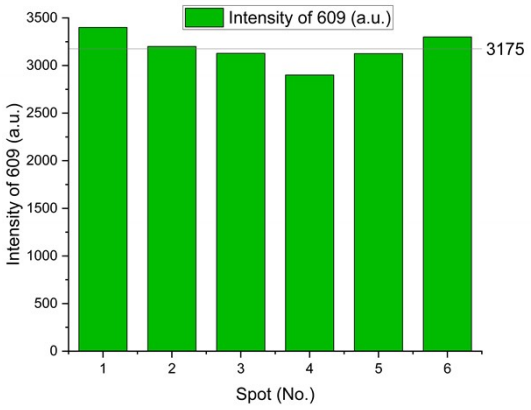

Fig. S7. The intensity at 609 cm^{-1} peak of R6G on six SERS MoO_x substrates which fabricated under the same condition.

Table S5: SERS intensity of R6G at 609 cm^{-1} peak absorbing on six MoO_x SERS substrates which fabricated under the same condition

No.	1	2	3	4	5	6
Intensity (a.u.)	3400	3200	3128	2900	3125	3300
Summary						
Count	Sum	Average	SD	RSD (%)		
6	19053	3175.5	171.58526	5.38		

Table S6: SERS intensity of R6G at 609 cm^{-1} peak at five random positions with 1 ppm adsorbed on the surface of MoO_x SERS substrate produced after 3 months, 6 months, and 9 months.

No.	3 months	6 months	9 months
1	3000	3200	3100
2	3100	2950	3200
3	2800	3257	2500
4	3500	2400	2800
5	3200	2784	2700

Summary					
Sample	count	sum	average	SD	RSD (%)
3 months	5	15600	3120	258.84358	8.23
6 months	5	14591	2918	347.04063	11.89
9 months	5	14300	2860	482.70074	13.32