Supporting Information

Synthesis and photothermal performance of non-stoichiometric molybdenum oxide (MoO_{3-x}) prepared by gamma radiation

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Summary

Structural advancing of MoO_3 with the γ-dose

From the analysis of X-ray diffractograms, it's possible to assess the evolution of exfoliation in the structure of α-MoO_3, as a function of γ-dose. The orthorhombic structure of α-MoO_3 has the preferred planes of greater intensity (020) with lattice parameters, a = 3.787 Å, b = 13.686 Å, and c = 3.787 Å. Depending on the dose of gamma radiation and the solvent used, advances in lattice parameters are verified. From the verification of the diffraction angles in the planes (020) it is possible to calculate the advance of the associated interplanar distances (d) by equation S1, which describes Bragg's law.[1]

$$2d_{hkl}sen\theta = n\lambda \qquad \text{(Eq. S1)}$$

Where d_{hkl} is the interplanar distance, θ is Bragg's angle, *n* is the order of diffraction (n = 1), and λ is the wavelength of the X-ray used (here, $Cu\ k_\alpha$ λ = 1.5406 Å).

Considering that there is no change in the crystalline structure, the lattice parameters (a, b, and c) can be calculated, from the d_{hkl} values presented in Table S1 for water, Table S2 for formic acid, and Table S3 for DMF, using the equation 2.

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \qquad \text{(Eq. S2)}$$

The average crystallite size (D) as well as the inter-planar spacing between atoms (d-spacing) of the MoO_3. For the samples were calculated by the Scherrer relation (Eq. 3).[2]

$$D = \frac{0.9\lambda}{\beta cos\theta} \qquad \text{(Eq. S3)}$$

Where k is the shape factor with value k = 0.94, β is the full width at half maxima (FWHM) for the plane (020), and θ is the Bragg's angle.

Due to the exfoliation process, the structure it's susceptible to lattice strains (ξ), which was calculated by the Wilson formula (Eq. S4). That given information about imperfection and distortion in the crystal structure.[3,4] The dislocation density associated with the displacement of atoms from the ideal position was calculated using the Equation S5.[5]

$$\xi = \frac{\beta_{hkl}}{4tan\theta_{hkl}} \qquad \text{(Eq. S4)}$$

$$\delta_{dis} = \frac{1}{D^2} \qquad \text{(Eq. S5)}$$

Table S1 Water PXRD parameters

Dose (kGy)	$2\theta_{(020)}$	Lattice parameter (Å)			Interplanar distance d, (nm)	Cell Volume (Å^3)	Crystallite size, D (nm)	Dislocation Density δ_{dis} (× 10^{-4} lines/nm)	Lattice strain, ξ (× 10^{-3})
		a	b	c					
0	12.94	3.78	13.68	3.25	0.68	168.33	57.41	3.03	5.27
30	12.83	3.80	13.80	3.26	0.69	170.94	76.28	1.72	3.26
60	12.81	3.80	13.80	3.26	0.69	170.96	71.69	1.94	3.03
90	12.79	3.80	13.82	3.26	0.69	171.32	67.13	2.22	4.05

Table S2 FA PXRD parameters

Dose (kGy)	$2\theta_{(020)}$	Lattice parameter (Å)			Interplanar distance d, (nm)	Cell Volume (Å^3)	Crystallite size, D (nm)	Dislocation Density δ_{dis} (× 10^{-4} lines/nm)	Lattice strain, ξ (× 10^{-3})
		a	b	c					
0	12.94	3.78	13.68	3.25	0.68	168.33	57.41	3.03	5.27
30	12.89	3.79	13.80	3.25	0.69	170.67	68.80	2.11	4.98
60	12.85	3.80	13.78	3.26	0.69	170.66	73.80	1.83	3.02
90	12.82	3.80	13.83	3.26	0.69	171.28	65.66	2.32	2.91

Table S3 DMF PXRD parameters

Dose (kGy)	$2\theta_{(020)}$	Lattice parameter (Å)			Interplanar distance d, (nm)	Cell Volume (Å^3)	Crystallite size, D (nm)	Dislocation Density δ_{dis} (× 10^{-4} lines/nm)	Lattice strain, ξ (× 10^{-3})
		a	b	c					
0	12.94	3.78	13.68	3.25	0.68	168.33	57.41	3.03	5.27
30	12.83	3.800	13.79	3.25	0.69	170.70	61.75	2.62	4.73
60	12.80	3.801	13.82	3.25	0.69	171.01	57.56	3.02	3.96
90	12.79	3.802	13.82	3.23	0.69	171.18	58.28	2.94	3.27

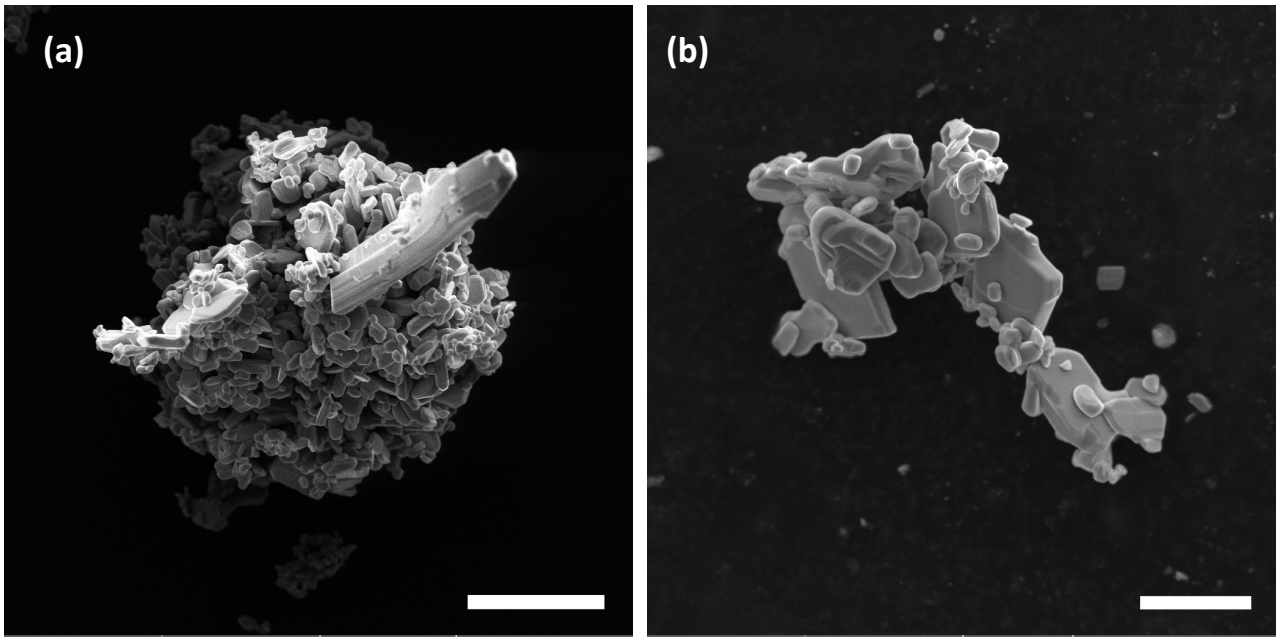

Fig. S1 SEM images of MoO_{3-x} water 90 kGy (a) scale bar 20 μm, and (b) scale bar 10 μm.

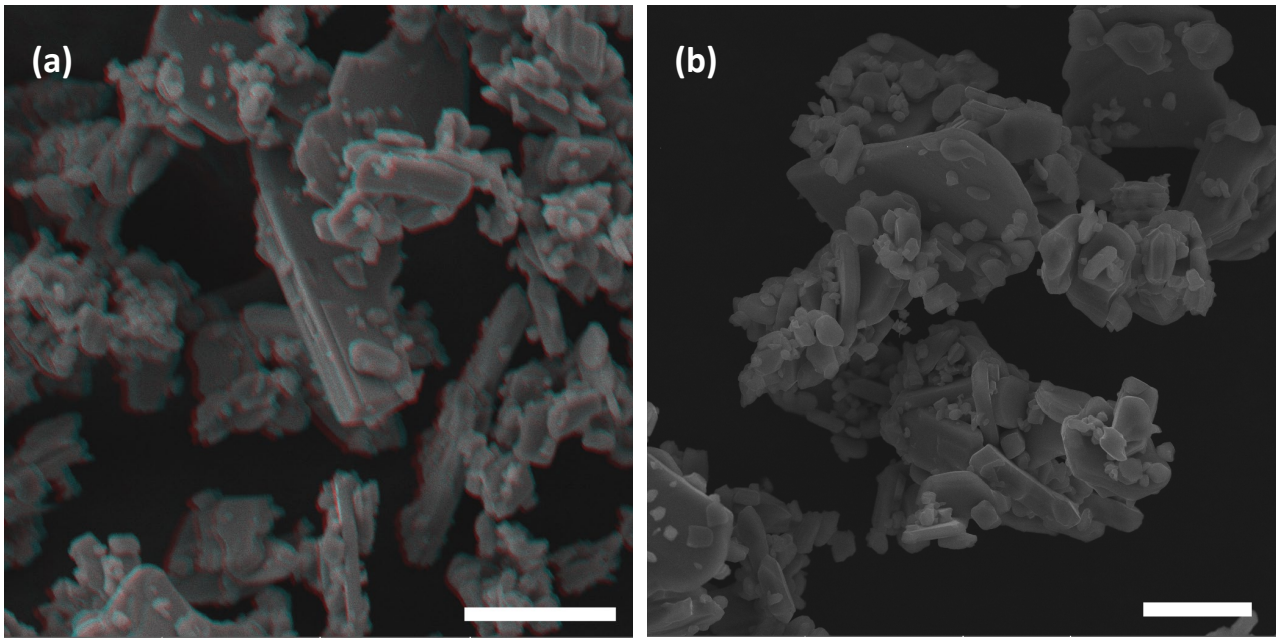

Fig. S2 SEM images of MoO_{3-x} DMF 90 kGy: (a) 3D image (required 3D glass) scale bar 20 μm, and (b) scale bar 10 μm.

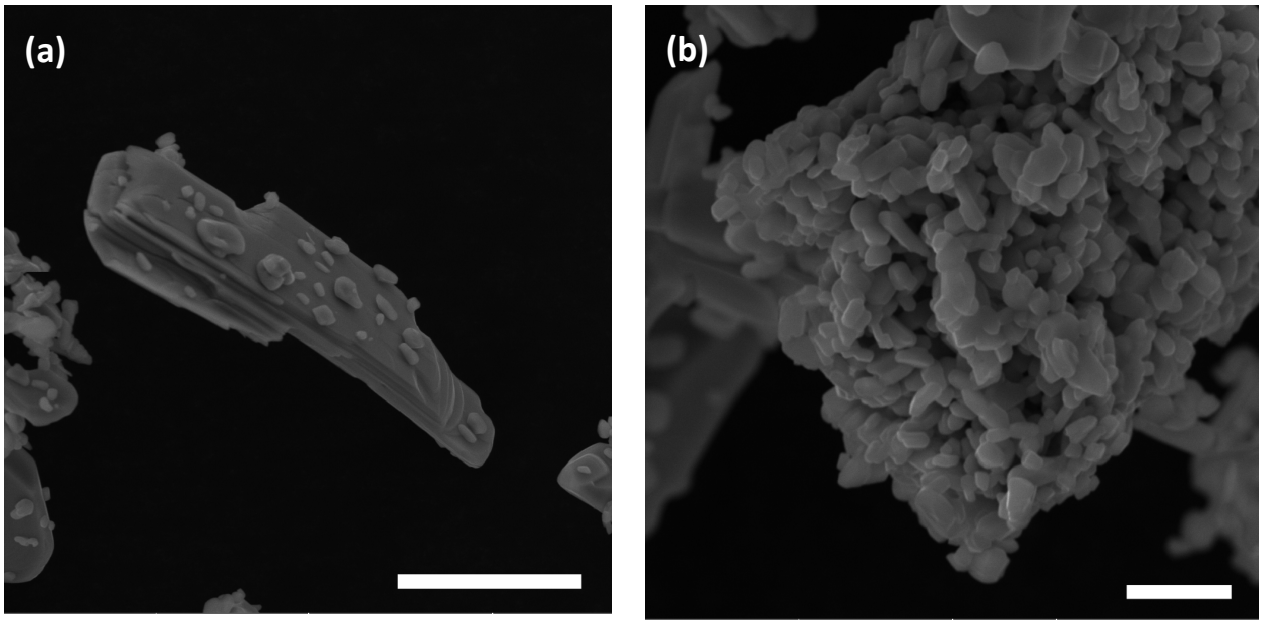

Fig. S3 SEM images of MoO_{3-x} FA 90 kGy (a) scale bar 20 μm, and (b) scale bar 5 μm.

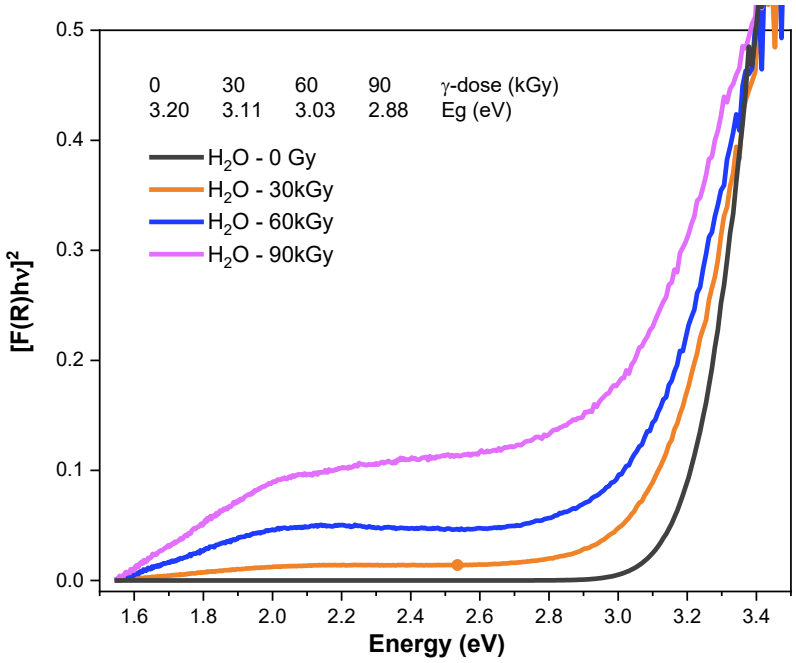

Fig S4 Tauc plot for water-MoO_{3-x}

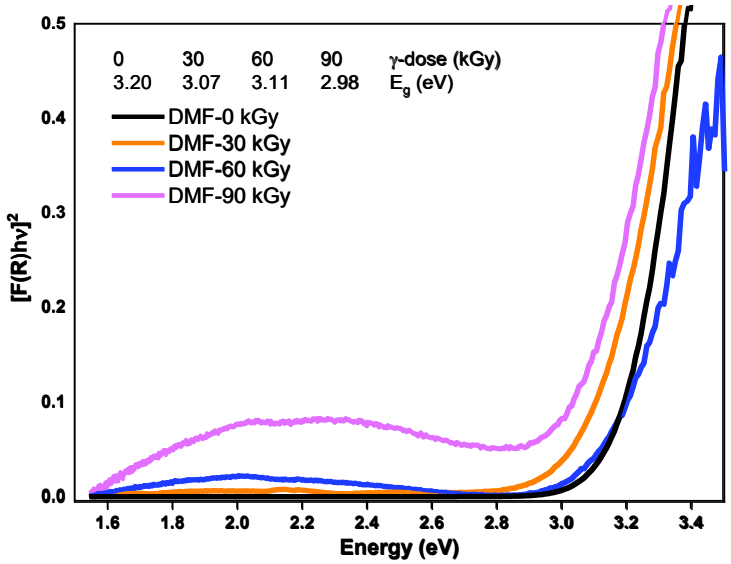

Fig S5 Tauc plot for DMF-MoO_{3-x}

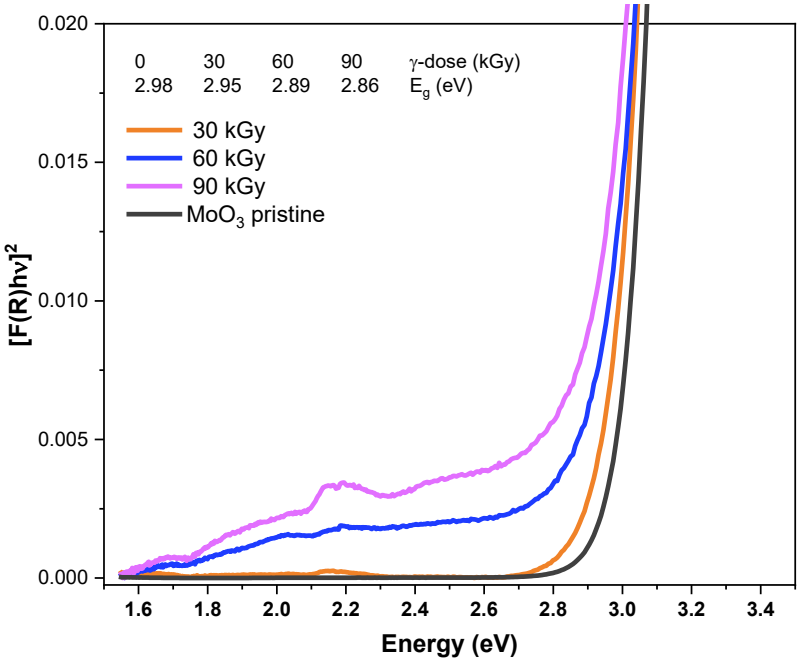

Fig S6 Tauc plot for FA-MoO_{3-x}

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