Supplementary Information (SI) for Journal of Materials Chemistry C.

A Delve into Bandgap Tuning and Nonlinear Optical Properties of Hydrothermally Synthesized Pristine and Boron Doped Molybdenum trioxide Nanorods

Anjali G[1,2], Mallikarjun Anandalli[2], Kala M S[1,*], Nandakumar Kalarikkal[2,3,4,*]

[1] Department of Physics, St. Teresa's College, Ernakulam, Kerala-682011, India

[2]International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, Kerala-686560, India

[3]School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam, Kerala-686560, India

[4]International Centre for Ultrafast Studies, Mahatma Gandhi University, Kottayam, Kerala-686560, India

Supplementary information

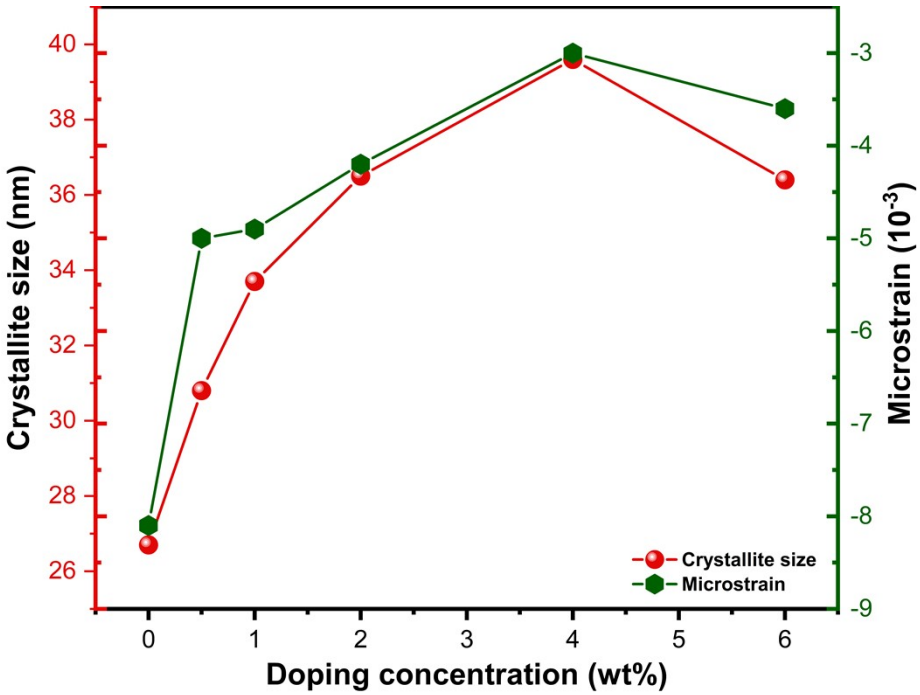

Figure S 1: Correlation graph of crystallite size and microstrain with doping concentration of boron

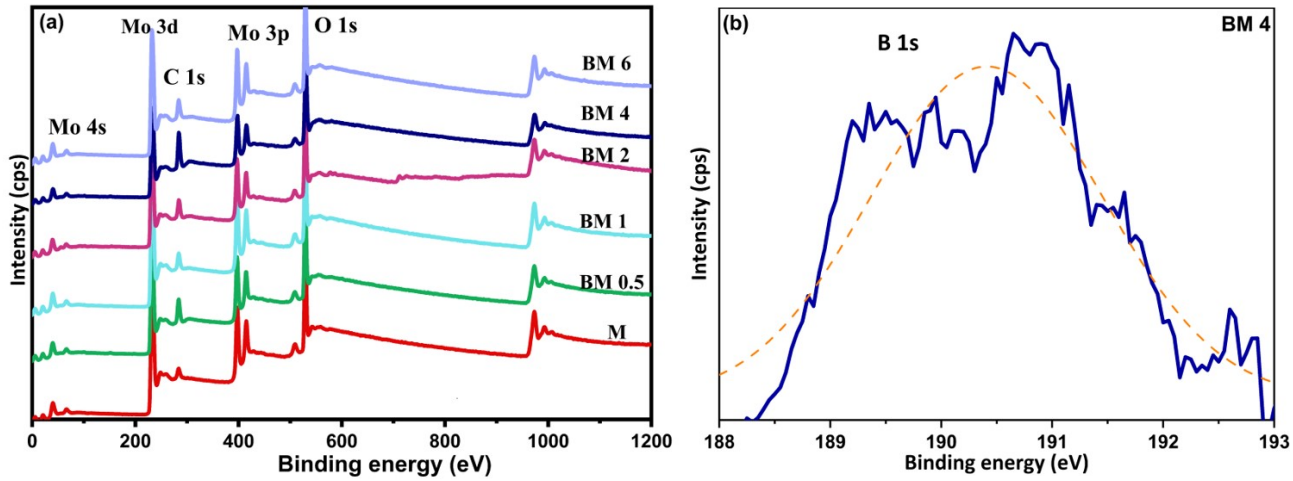

Figure S 2: (a)Full range XPS survey of MoO_3 and B-MoO_3 samples (b) B 1s spectra of BM 4 sample

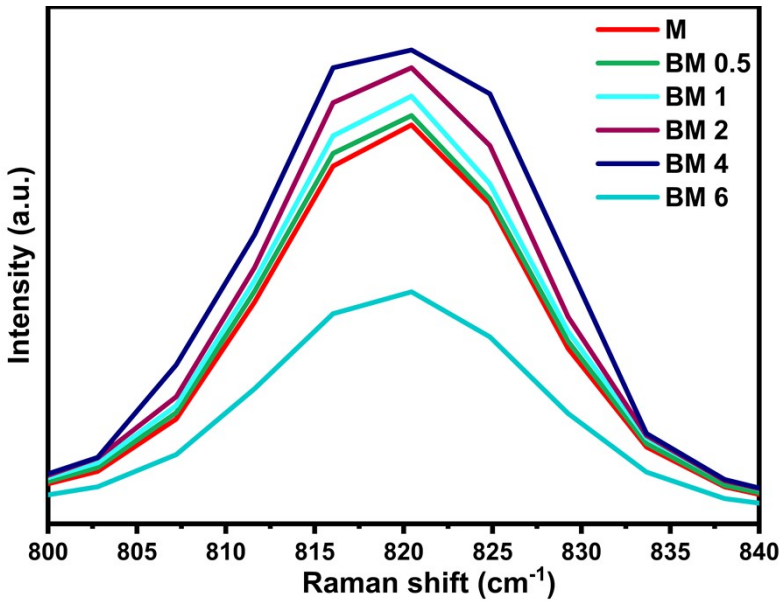

Figure S 3: Raman spectra peak corresponding to vibrational mode at 818cm^{-1} of pristine and doped MoO_3 (for finding the phonon profile)

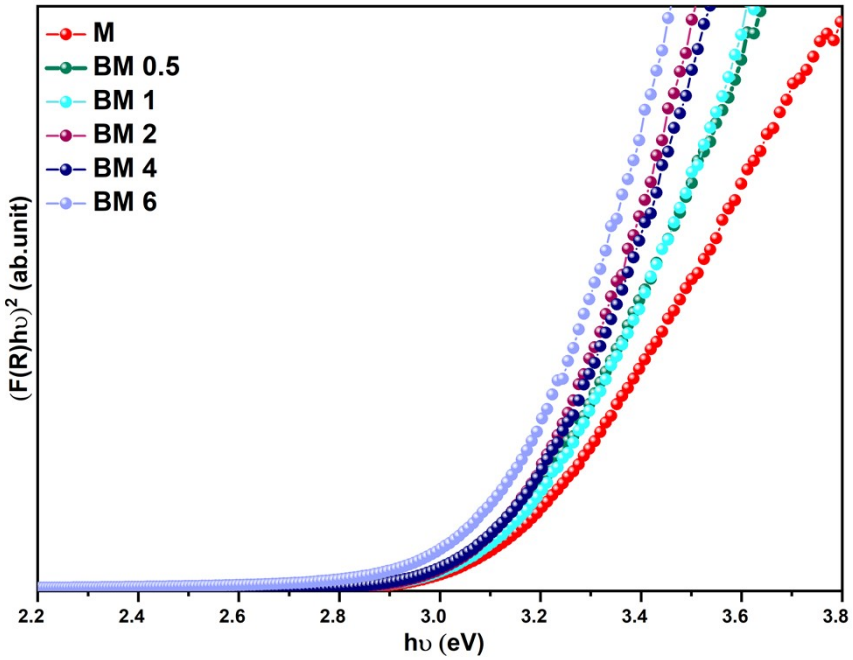

Figure S 4: Kubelka-Munck plot for finding the direct band gap of MoO_3 and B-MoO_3

Table S 1: Color coordinate parameters of the samples from the CIE diagram

Samples	Color Coordinates		Dominant wavelength (nm)	Color purity
	x	y		
M	0.1620	0.0582	459.9	90.6 %
BM 0.5	0.1617	0.0562	459.5	91 %
BM 1	0.1659	0.0605	458.7	89.3 %
BM 2	0.1710	0.0652	457.7	87.3 %
BM 4	0.1856	0.0602	448.5	84.3 %
BM 6	0.1604	0.0674	462.9	89.1 %

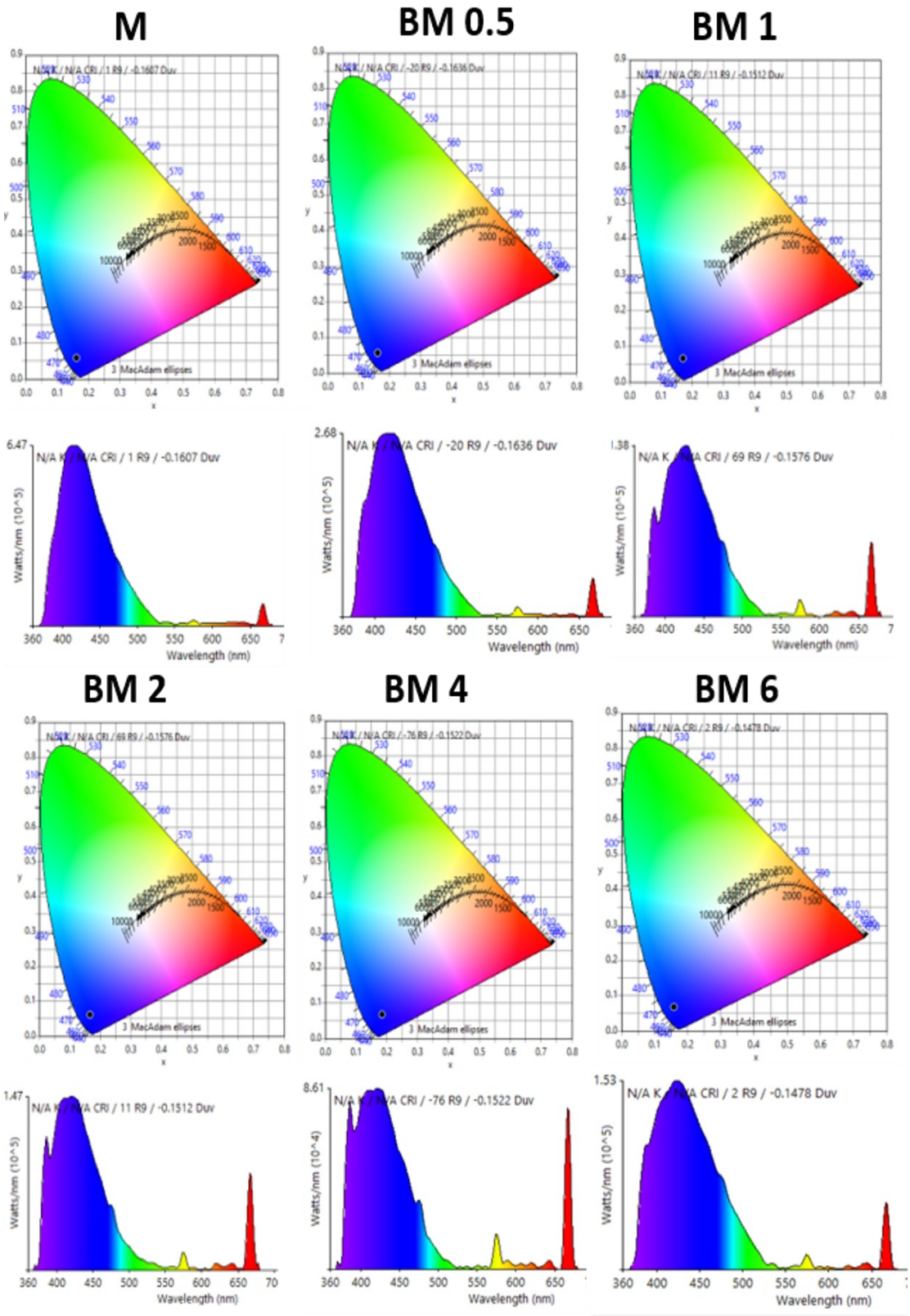

Figure S 5: CIE diagram and spectral irradiance curve of MoO_3 and B-MoO_3 samples

Time Resolved Fluorescence Study

The PL life time (τ) of the sample can be defined as the time at which intensity emission reaches 1/e and the fluorescence decay curve can be fitted using tri-exponential kinetics equation.

$F(t)= A + B_1 \exp(-t/\tau_1) + B_2 \exp(-t/\tau_2) + B_3 \exp(-t/\tau_3)$

The fitted parameters and average life time were given in Table S 2.

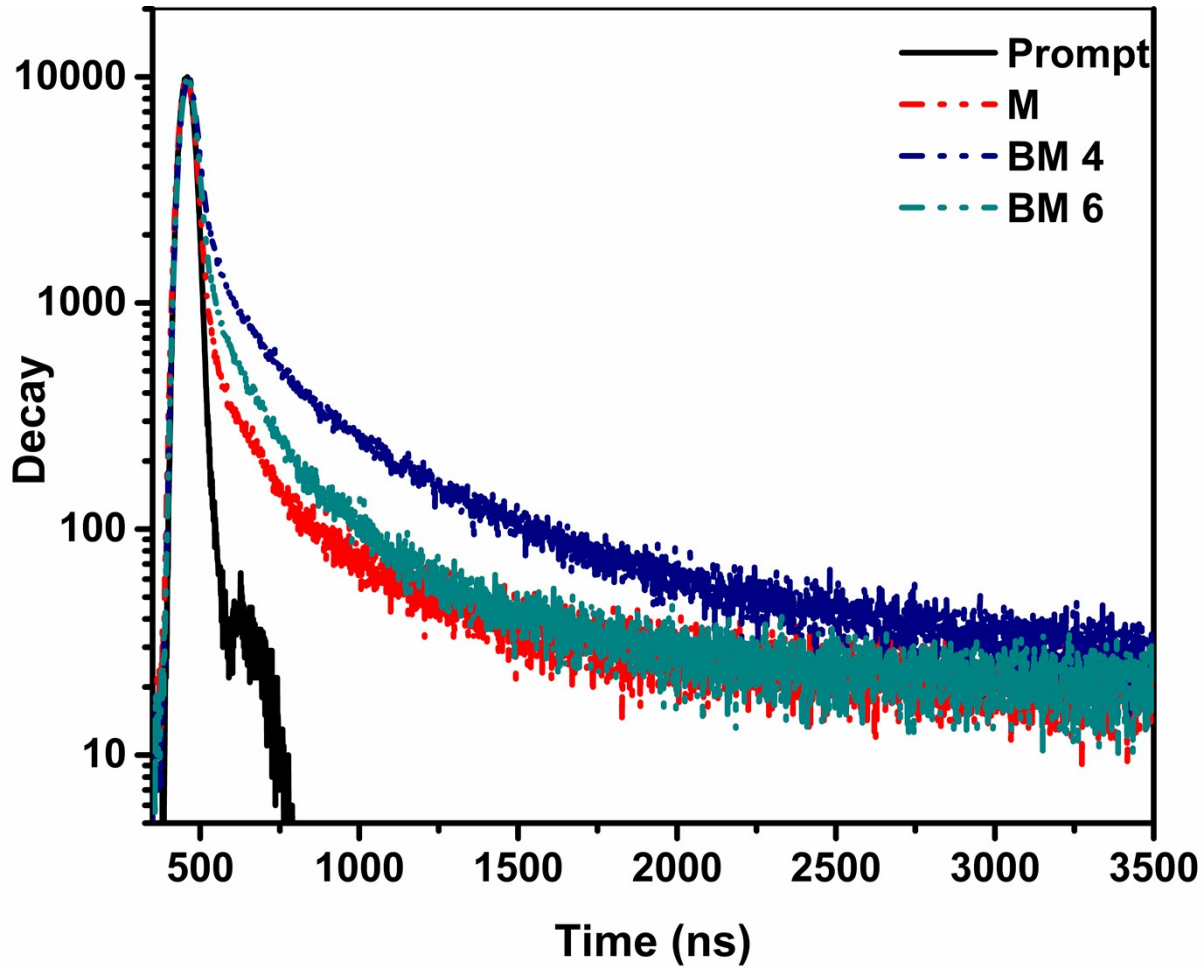

Figure S 6: Decay curve of MoO_3 and B-MoO_3 (BM 4 and BM 6) from time-resolved fluorescence study

All the samples show the mono-exponential decay curve with an average lifetime in the range of 1.8 -11. The BM 4 sample has greater life time over other samples. As explained in the

photoluminescence part, the increase in doping concentration can introduce defect levels that can act as trapping centers for charge carriers by preventing recombination. This results in an increase in the lifetime of charge carriers at excited levels. This, in turn, can enhance the sequential two-photon absorption in doped samples.

Table S 2: Fitting parameters of fluorescence decay curves performed by time-resolved fluorescence spectroscopy technique

Sample	T1(ns)	T2(ns)	T3(ns)	B1	B2	B3	τ_{ave} (ns)
M	2.47	0.23	13.6	1.73×10^{-3}	0.121	2.61×10^{-4}	1.8
BM 4	4.64	17.4	1.07	858.61	352.14	625.81	11
BM 6	2.79	12.1	0.27	2.82×10^{-3}	4.37×10^{-4}	0.102	2

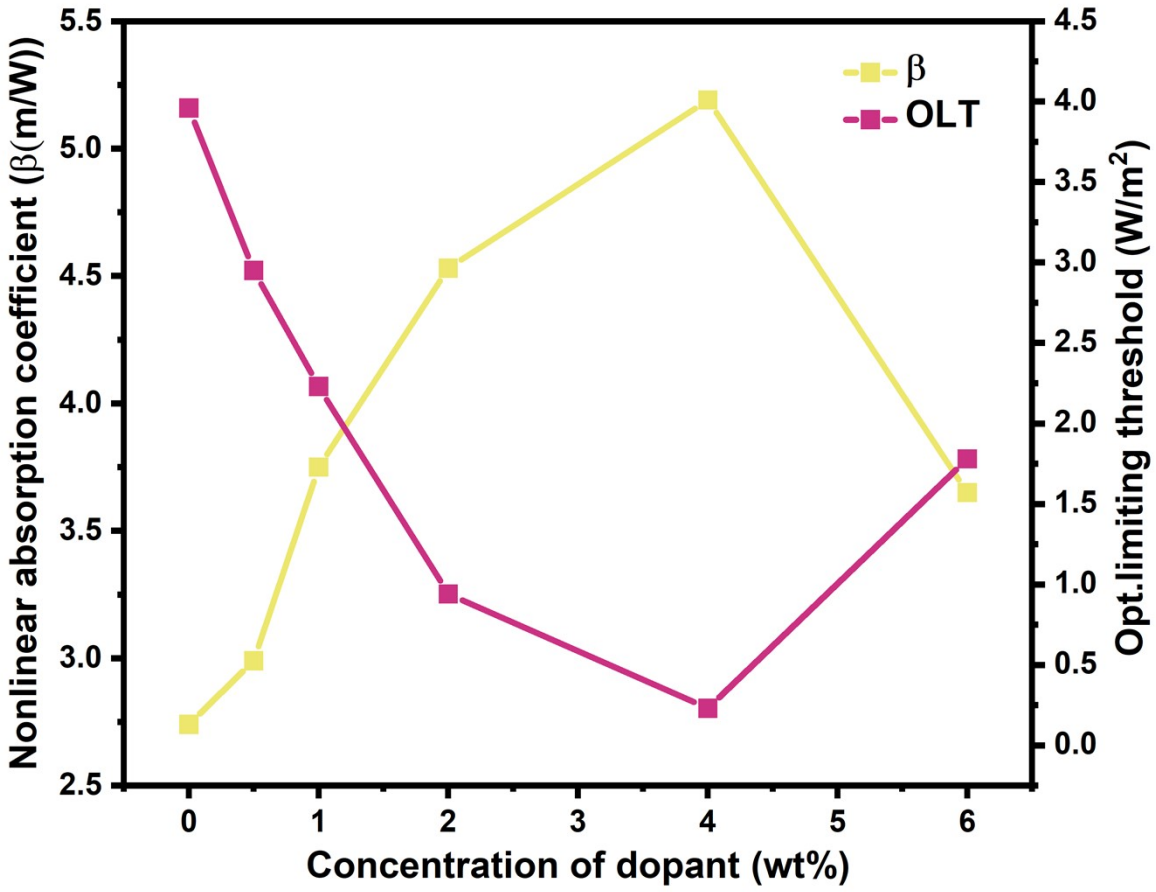

Figure S 7: Correlation graph of nonlinear absorption coefficient and optical limiting threshold value with concentration of boron doping