

Visible Light Photodegradation of Dyes and Paracetamol by Direct Sensitization Mechanism onto *Metallic* MoO₂ Nanocrystals

Alessandro Di Mauro,¹ Marta Maria Natile,² Anton Landström,³ Isabella Concina,³ Matteo Ferroni,⁴
Vittorio Privitera,¹ Giuliana Impellizzeri,¹ Mauro Epifani^{5,*}

¹ CNR-IMM, Via S. Sofia 64, 95123 Catania, Italy;

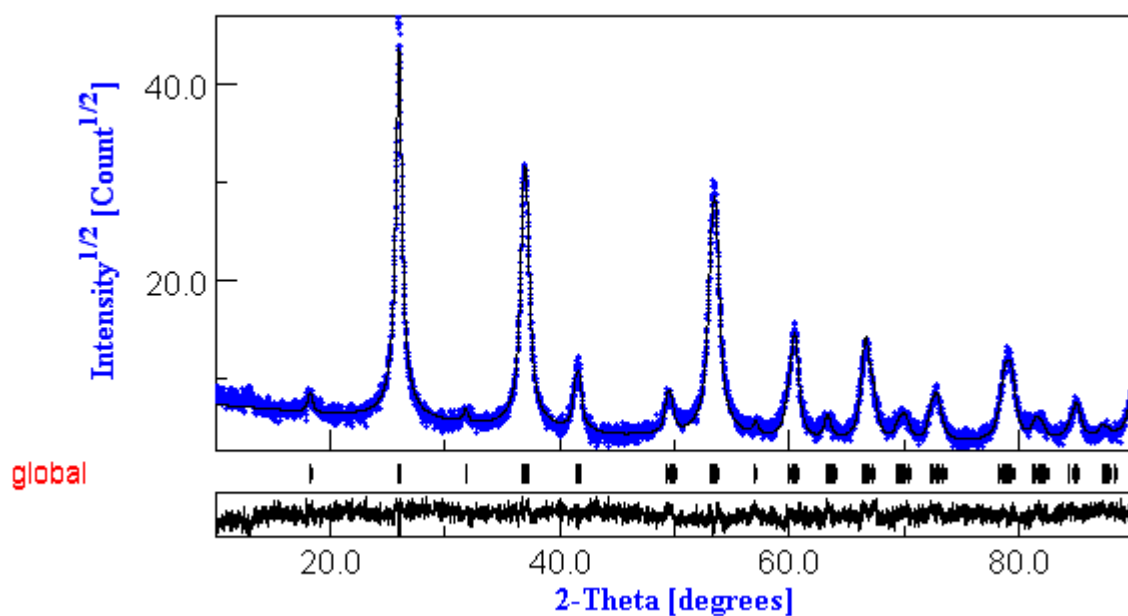
² Istituto di Chimica della Materia Condensata e Tecnologie per l'Energia, Consiglio Nazionale delle Ricerche (ICMATE-CNR) and Dipartimento di Scienze Chimiche, Università di Padova, Via F. Marzolo 1, 35131 Padova, Italy;

³ Luleå University of Technology, 971 87 Luleå, Sweden;

⁴ Department of Information Engineering, University of Brescia, Via Branze, Brescia, Italy and CNR-IMM, Via Gobetti, Bologna, Italy;

⁵ CNR-IMM, Via Monteroni c/o Campus Universitario, 73100 Lecce, Italy

*maurosalvatore.epifani@cnr.it



Name	Value	Min	Max	Error	Status	Output
● _pd_spec_size_radius	0	0.0	0.0	0.0	Fixed	false
● _pd_spec_size_radius_y	0	0.0	0.0	0	Fixed	false
📁 layer1	-	-	-	-	*****	false
📁 DataFileSet_x	-	-	-	-	*****	false
📁 global	-	-	-	-	*****	false
● _cell_length_a	5.630473	5.0	30.0	3.96666...	Refined	false
● _cell_length_b	4.851831	5.0	30.0	5.09651...	Refined	false
● _cell_length_c	5.6195307	5.0	30.0	6.41536...	Refined	false
● _cell_angle_beta	120.67191	90.0	120.0	0.00540...	Refined	false
● _riet_par_strain_thermal	0	-0.1	0.1	0	Fixed	false
● _exptl_absorpt_cryst_size	0	0.001	100.0	0	Fixed	false
● _riet_par_phase_scale_factor	1.0	0.0	100.0	0	Fixed	false
📁 Isotropic	-	-	-	-	*****	false
● _riet_par_cryst_size	289.7034	50.0	5000.0	1.5932544	Refined	false
● _riet_par_rs_microstrain	0.0010881434	0.0	0.005	7.97675...	Refined	false
📁 Atomic Structure	-	-	-	-	*****	false

Figure S1. Rietveld refinement carried out with the Maud software of the XRD pattern of the MoO₂ sample prepared by solvothermal treatment at 250 °C in oleic acid.

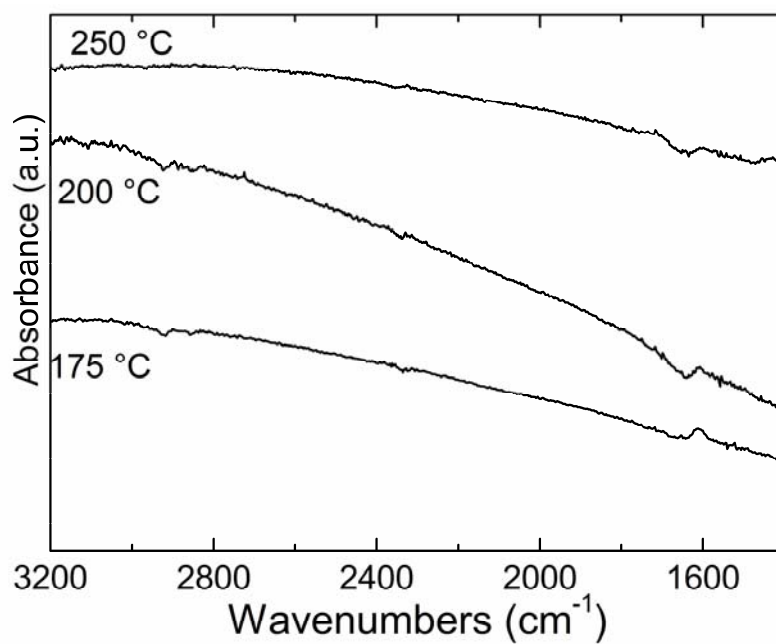


Figure S2. High frequency range of the FTIR spectra shown in Figure 5 of the manuscript.

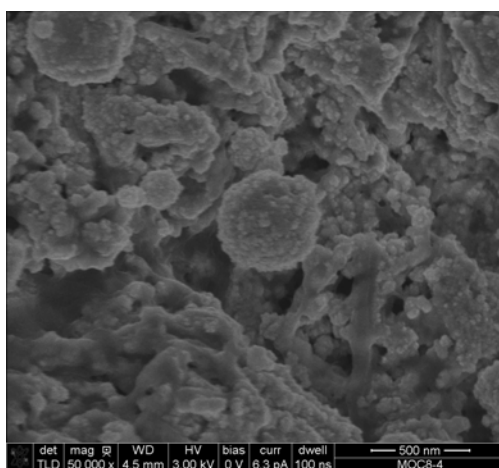


Figure S3-A: SEM image of the MoO₂ sample prepared after solvothermal treatment for 2h in oleic acid at 250 °C.

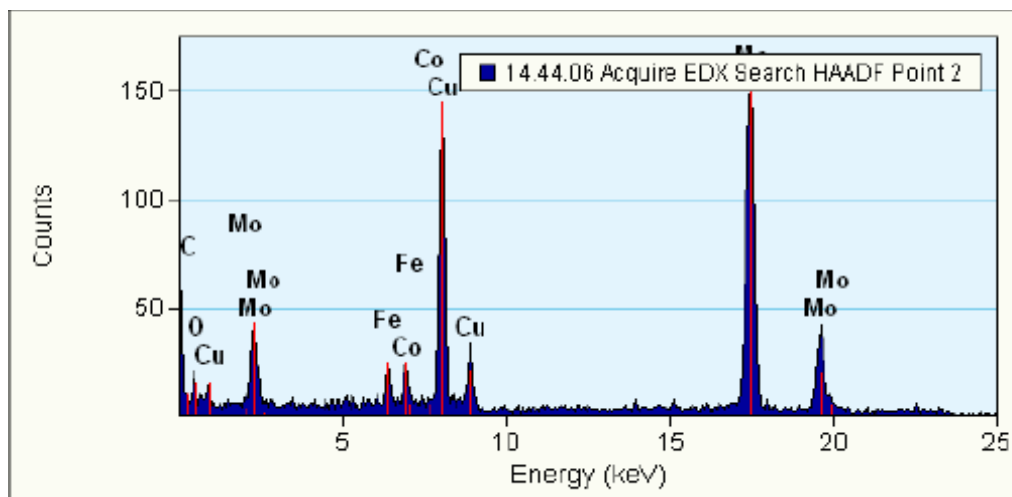


Figure S3-B. EDS data of the MoO_2 sample prepared after solvothermal treatment for 2h in oleic acid at 250 °C. Cu is a standard artefact owing to the TEM Grid. Fe/Co come from the bore of TEM lenses.

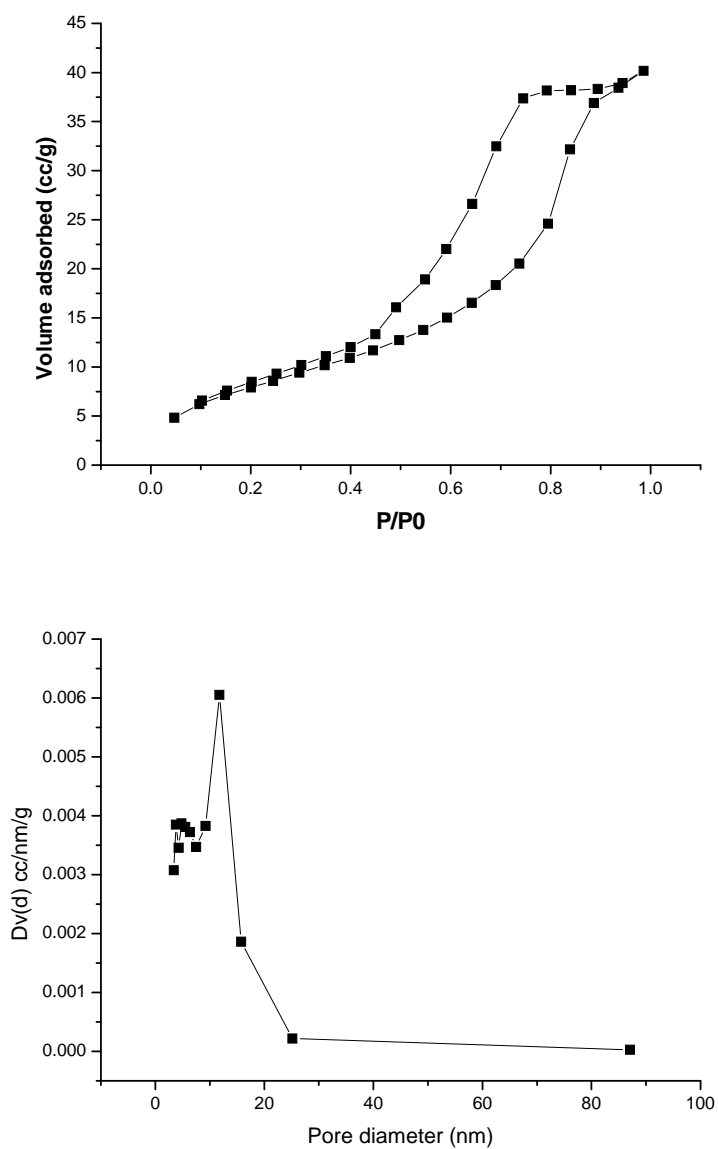


Figure S4. Adsorption/desorption isotherms (top) and pore size distribution (bottom) of the MoO₂ sample prepared after solvothermal treatment for 2h in oleic acid at 250 °C.

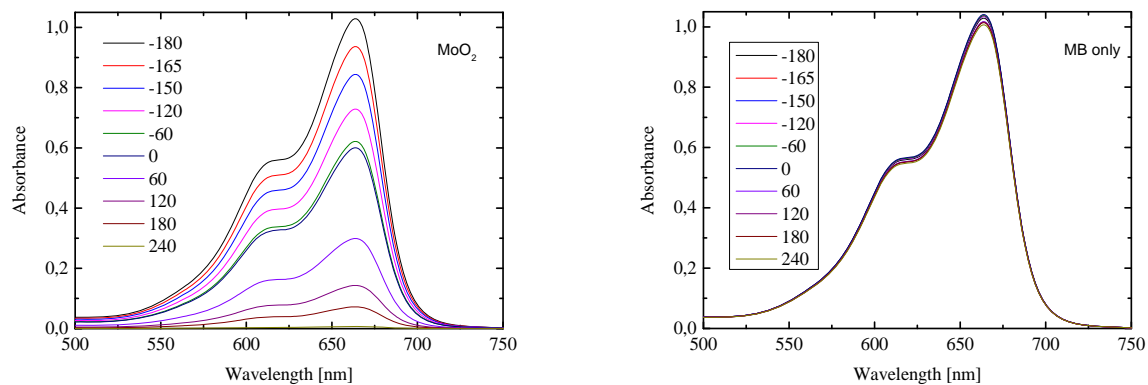


Figure S5. Absorption spectra of MB solutions for different adsorption times on MoO₂ and without MoO₂.

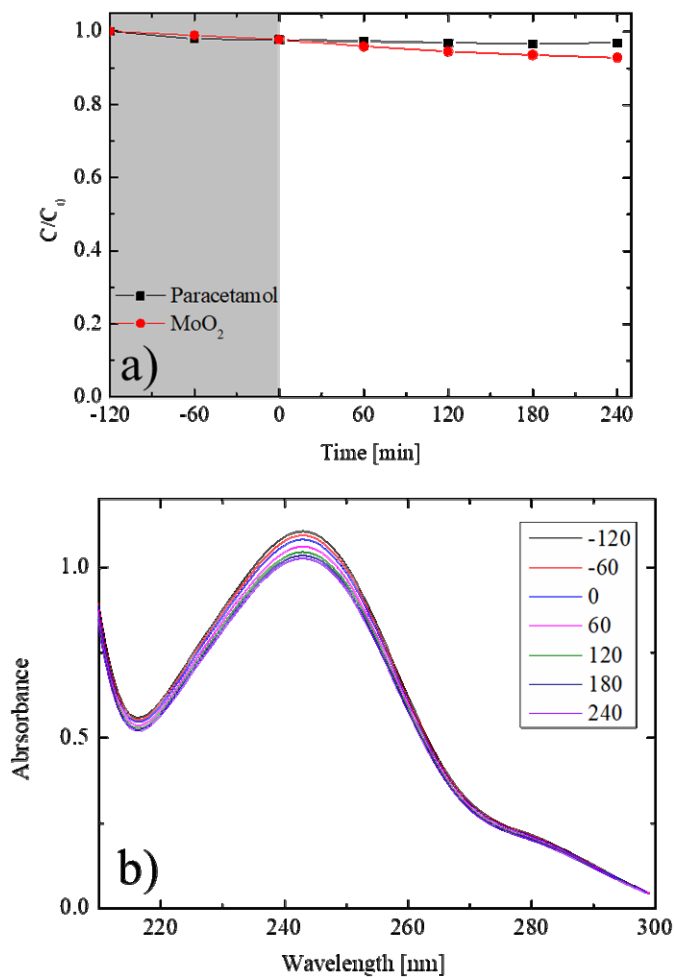


Figure S6. Paracetamol degradation under visible light, trend of degradation (a) and Spectra (b).

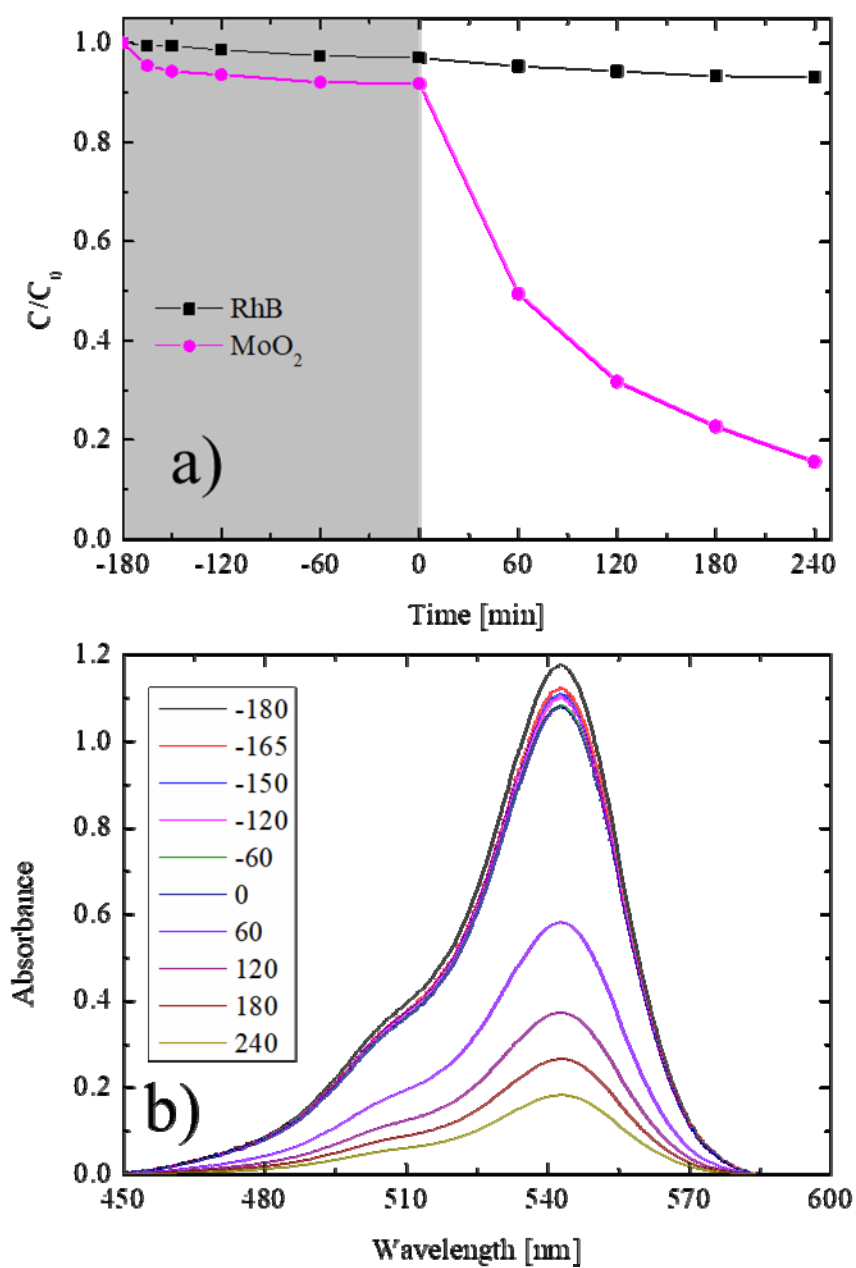


Figure S7. Rhodamine B degradation under visible light, trend of degradation (a) and Spectra (b).

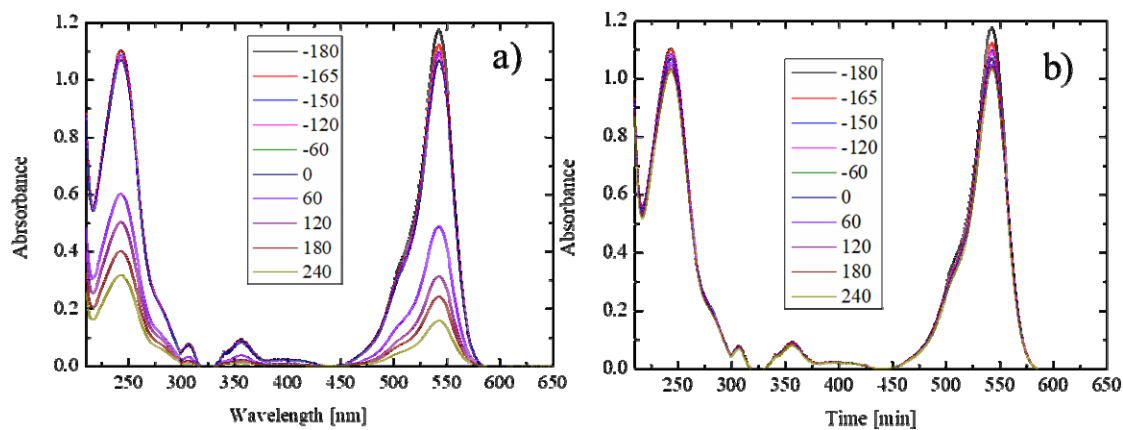


Figure S8 Assessment of dye-sensitization of paracetamol in presence of RhB using total visible spectrum (a) and a reduced spectrum (500-600 nm deducted) (b)