

Supplementary Information

Rare-Earth Modified Titania Nanoparticles: Molecular insight into Synthesis and Photochemical Properties

*Fredric G. Svensson¹, Bogdan Cojocaru^{*2}, Zhen Qiu³, Vasile Parvulescu², Tomas Edvinsson³,
Gulaim A. Seisenbaeva¹, Carmen Tiseanu⁴, and Vadim G. Kessler^{*1}*

¹Department of Molecular Sciences, Swedish University of Agricultural Sciences, Box 7015, SE-75007 Uppsala, Sweden.

²Department of Chemistry, University of Bucharest, B-dul Regina Elisabeta, nr. 4-12, RO-030018 Bucharest, Romania.

³Department of Materials Science & Engineering, Box 53, Uppsala University, SE-75103 Uppsala, Sweden.

⁴National Institute for Laser, Plasma and Radiation Physics (NILPR), RO-76900 Bucharest-Magurele, Romania.

*Correspondence: Vadim G. Kessler: vadim.kessler@slu.se; Bogdan Cojocaru: bogdan.cojocaru@chimie.unibuc.ro

Elemental mapping

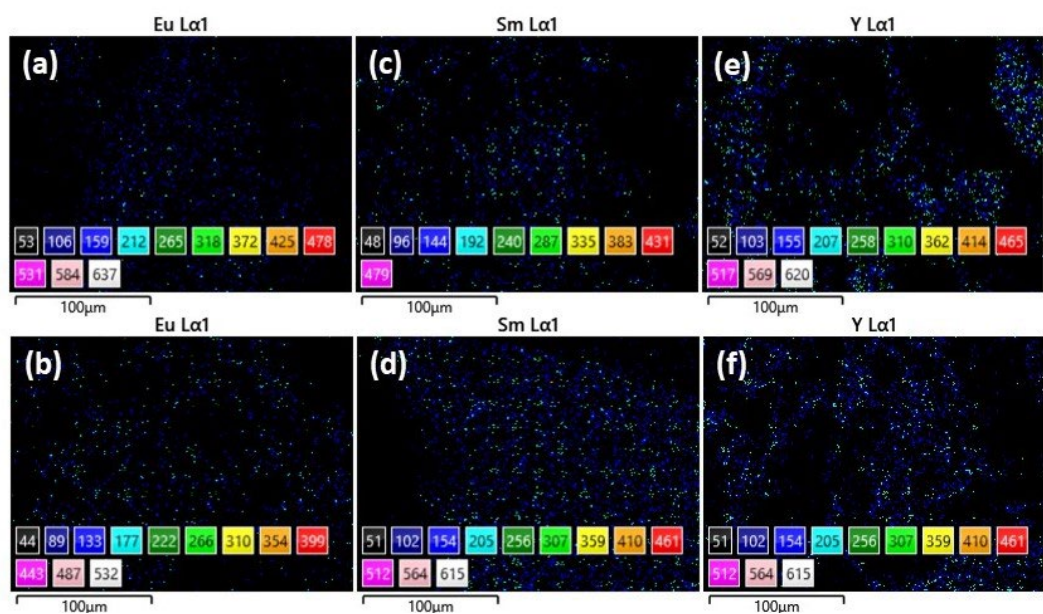


Figure S1. Elemental mapping of REE-modified titania nanopowders for Sm and Eu. (a) Ti-Eu2.5-500, (b) Ti-Eu2.5-600, (c) Ti-Sm2.5-500, (d) Ti-Sm2.5-600, (e) Ti-Y2.5-500, (f) Ti-Y2.5-600.

AFM micrographs of Eu-modified titania

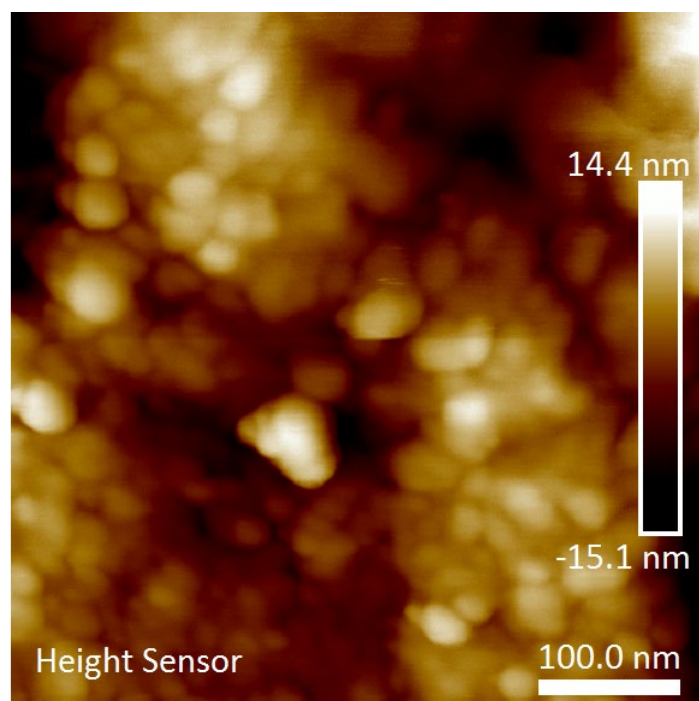


Figure S2. AFM micrograph of Ti-Eu2.5-500.

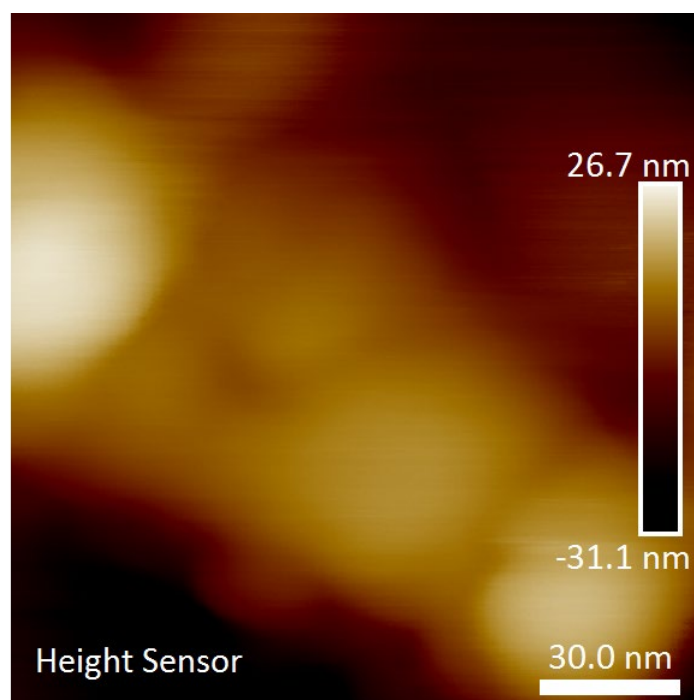


Figure S3. AFM micrograph of Ti-Eu5-700.

Supplementary Table S1. Bond lengths for Compound 1.

Bond	Length (Å)
Y1–O3	2.308(5)
Y1–O2	2.314(5)
Y1–O1	2.322(5)
Y1–O6	2.324(5)
Y1–O400(N4)	2.333(14)
Y1–O410(N4)	2.372(13)
Y1–O41(N4)	2.379(12)
Y1–O40(N4)	2.391(13)
Y1–O152(N2)	2.315(15)
Y1–O153(N2)	2.400(15)
Y1–O151(N2)	2.412(13)
Y1–O150(N2)	2.460(12)
Ti2–O8	1.754(5)
Ti2–O11	1.759(6)
Ti2–O1	1.979(5)
Ti2–O4	2.026(5)
Ti2–O3	2.145(5)
Ti2–O2	2.200(5)
Ti1–O7	1.747(5)
Ti1–O5	1.756(6)
Ti1–O6	1.968(5)
Ti1–O4	2.024(5)
Ti1–O3	2.148(5)

Ti1–O2	2.187(5)
O1–C1	1.452(9)
O2–C3A	1.463(10)
O3–C3	1.422(10)
O4–C4	1.463(10)
C1–C1B	1.477(15)
C1–C1A	1.495(14)
O6–C6	1.451(9)
C4–C4A	1.395(14)
C4–C4B	1.486(13)
O5–C5	1.517(12)
O8–C8	1.369(12)
O11–C11	1.434(12)
O7–C7	1.420(12)
C6–C6A	1.503(12)
C6–C6B	1.542(11)
C3D–C3A	1.546(13)

Supplementary Table S1. Continued.

Bond	Length (Å)
C8B–C8	1.458(15)
C8A–C8	1.282(19)
C7–C7B	1.427(14)
C7–C7A	1.458(14)
C3A–C3B	1.445(13)
C5–C5A	1.474(13)
C5–C5B	1.510(13)
C3–C30	1.448(15)
C3–C32	1.496(14)
C11A–C11	1.468(14)
C11–C11B	1.41(2)
O15C–N2	1.192(12)
O43–N4	1.191(10)
N4–O410	1.152(15)
N4–O400	1.167(17)
N4–O40	1.347(18)
N4–O41	1.440(18)
N2–O152	1.101(18)
N2–O151	1.52(2)
N2–O150	1.43(2)
N2–O153	1.082(17)
