

## The formation and effect of O-vacancies in doped TiO<sub>2</sub>

New Journal of Chemistry

Kaustava Bhattacharyya<sup>a,d\*</sup>, B. Modak<sup>c</sup>, C. Nayak<sup>b</sup>, R. G. Nair<sup>a</sup>, D. Bhattacharyya<sup>b,d</sup>, S. N. Jha,  
and A. K. Tripathi<sup>a,d</sup>

a- Chemistry Division, Bhabha Atomic Research Centre, Mumbai-40085, India

b- Atomic & Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai – 400  
085, India

c- Theoretical Chemistry Section, Bhabha Atomic Research Centre, Mumbai-40085, India

d- Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094

### Supplementary Information

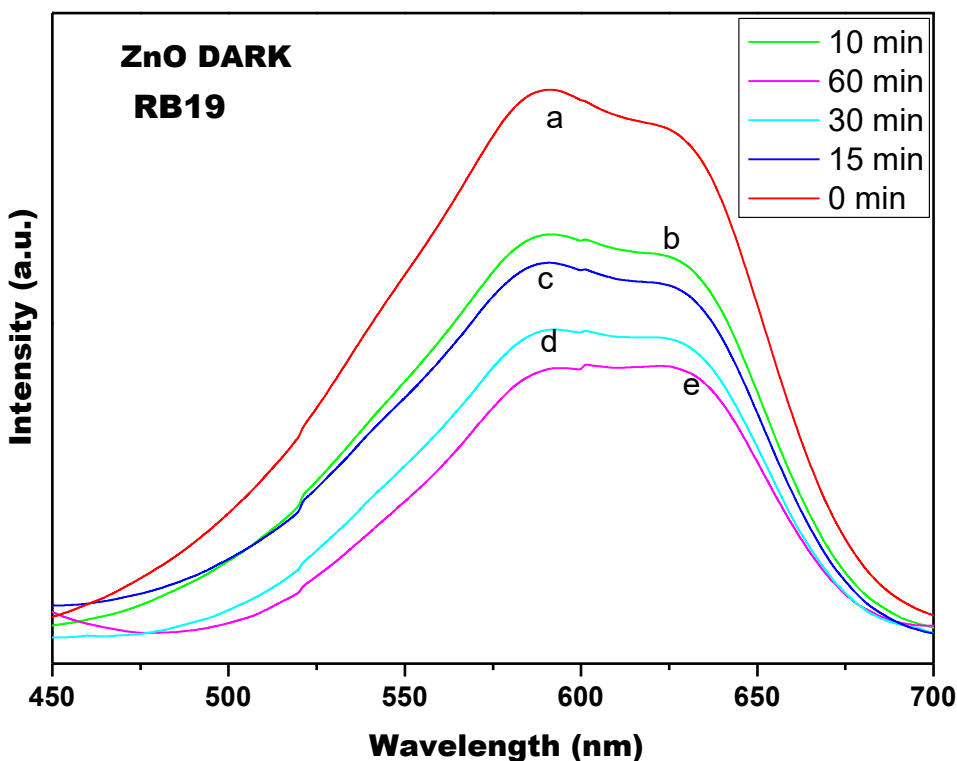


Fig. S.1:- Adsorption profile of RB-19 on nano- ZnO where the adsorption is carried out for a) 0 min, b) 10 min; c) 15 min; d) 30 min; e) 60 min.

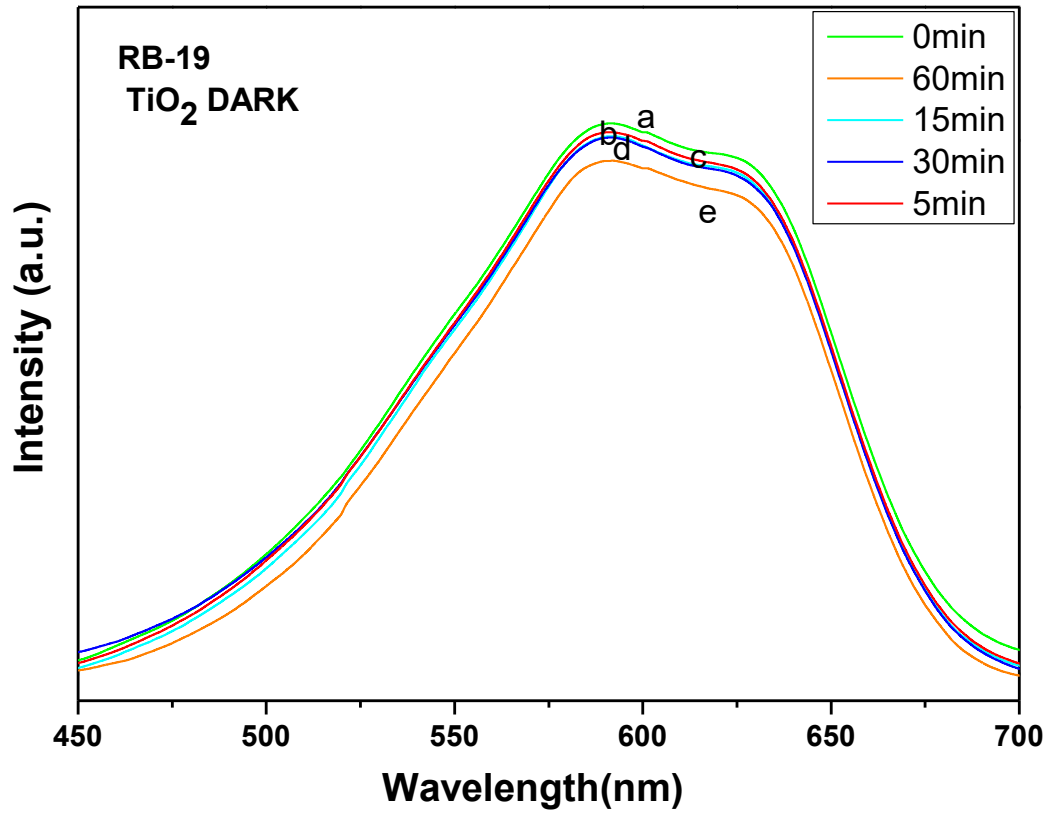


Fig. S.2:- Adsorption profile of RB-19 on nano- TiO<sub>2</sub> where the adsorption is carried out for a) 0 min, b) 10 min; c) 15 min; d) 30 min; e) 60 min.

Sample	Crystallite Size (nm) <sup>a</sup>	Surface Area (m <sup>2</sup> /g) <sup>b</sup>	a=b (Å)	c(Å)	Vol (Å <sup>3</sup> )	Composition from ICP-MS
TiO <sub>2</sub>	20	54.49	3.785	9.513	136.28	-
Zn-1	20	46.74	3.785	9.458	135.51	Ti=34.52, Zn=0.91
Zn-2	15	59.85	3.785	9.417	134.90	Ti=35.12, Zn=1.62
Zn-5	12	70.1	3.785	9.429	135.01	Ti=34.29, Zn=3.62
Zn-10	12	68.6	3.785	9.403	134.71	Ti=32.92, Zn=6.83

Table-S.I -1 : The table shows the crystallite size and the surface area of the different Zn-doped TiO<sub>2</sub> and nano TiO<sub>2</sub> particles. It shows the lattice cell parameters of a, b, c and the total volume of the Anatase lattice with different doping of Zn. The lattice parameters and the cell volume are calculated by the POWDEREX software

a: Crystallite size obtained from Scherer Equation from the XRD data (Fig. S.1) using the  $\theta = 25.4^\circ$ ;

b: Pore volume obtained from the BJH distribution plot of the desorption branch at  $p/p_0 \sim 0.995$