

Supporting Information

Experimental and Theoretical Insights into Influence of Hydrogen and Nitrogen Plasma on the Water Splitting Performance of ALD Grown TiO₂ Thin Films

Alexander Sasinska¹, Danny Bialuschewski¹, Mazharul M. Islam², Trilok Singh¹, Meenal Deo¹, and Sanjay Mathur^{1,*}

1) *Institute of Inorganic Chemistry, University of Cologne, Greinstrasse 6, Cologne-50939, Germany*

2) *Mulliken Center for Theoretical Chemistry, University of Bonn, Berlingstrasse 4–6, Bonn-53115, Germany*

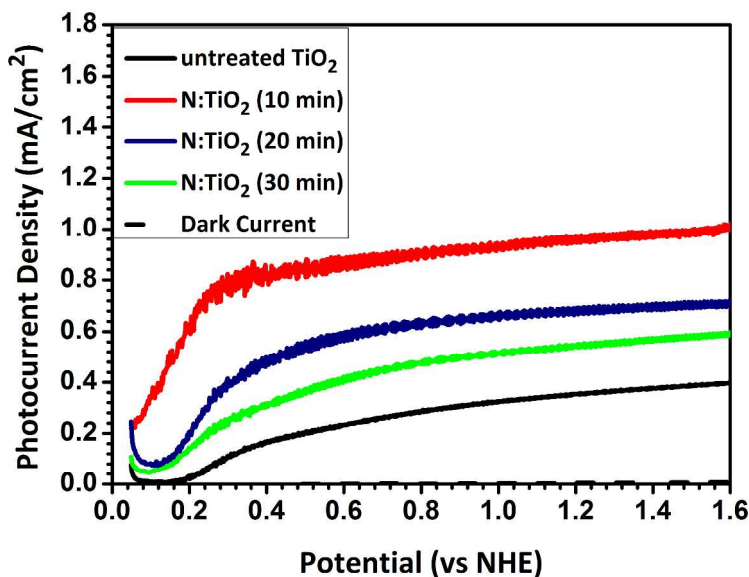


Figure S1: I-V curves of N₂ plasma treated TiO₂ for prolonged plasma exposure times.

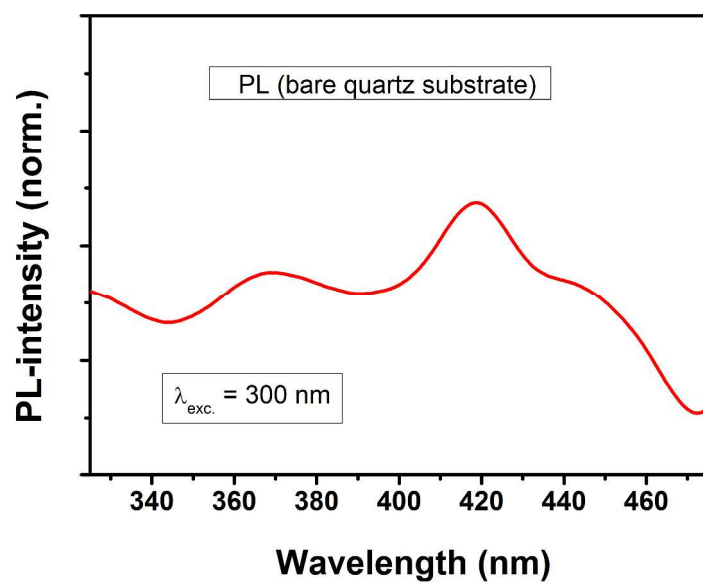


Figure S2: PL spectrum of bare quartz substrate.

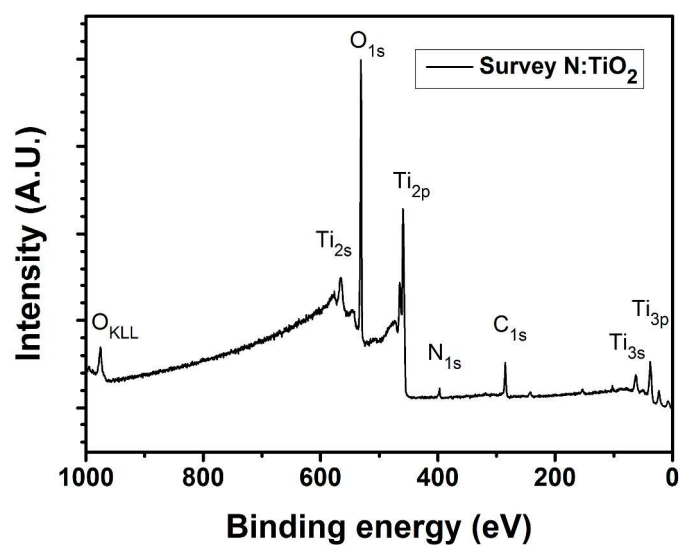


Figure S3: XPS survey spectrum of N₂ plasma treated TiO₂.

Table S1. Comparison of calculated structural parameters such as lattice parameters (Å) and bond distances (Å), and band gap (eV) with available experimental data.

		Calc.	Exp.
Lattice Parameter (Å)	<i>a</i>	3.774	3.782 (Ref. 66)
	<i>c</i>	9.522	9.502
Bond Distances (Å)	Ti(1) - O	1.929	1.932
	Ti(2) - O	1.979	1.979
Band Gap (eV)	E_g	3.3 eV	3.4 eV (Ref. 67)