

DEFECT ENGINEERING OF ATOMIC LAYER DEPOSITED TiO₂ FOR PHOTOCATALYTIC APPLICATIONS

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STM/STS



Nano-phase
Materials



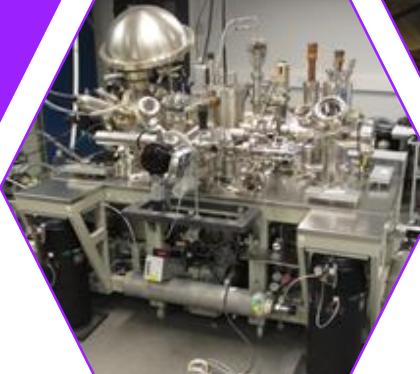
ALD

NanoESCA/XPEEM

Surface and
Interface
Physics



Electronic
structure



Multilab/XPS

Surface
Reactions



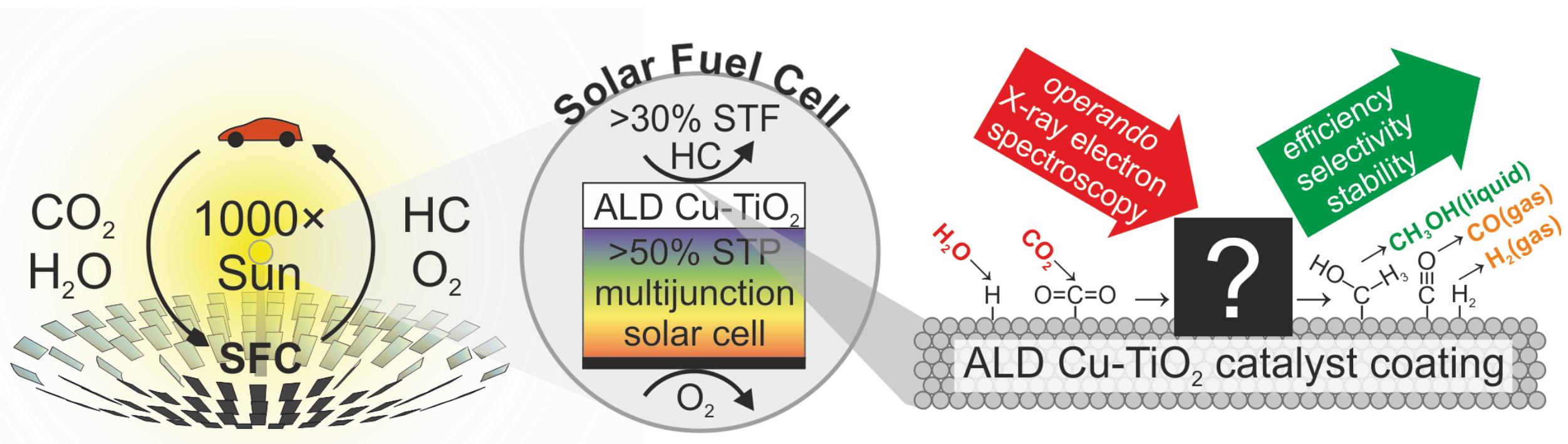
PEC
ICP-MS
GC

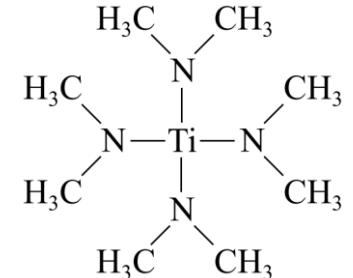
MAX IV Laboratory
Synchrotron Light



Solar Fuel Production

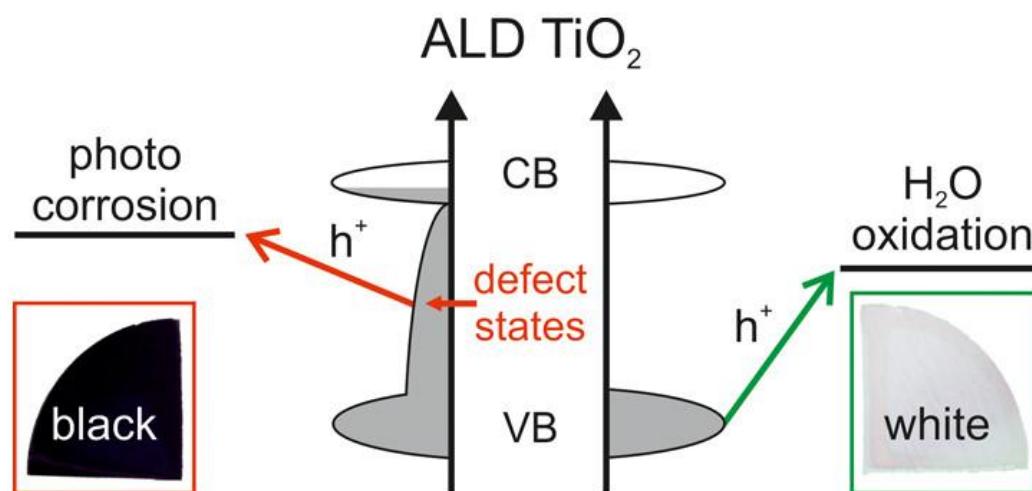
Research and development of photoactive materials and surface reactions for artificial photosynthesis.



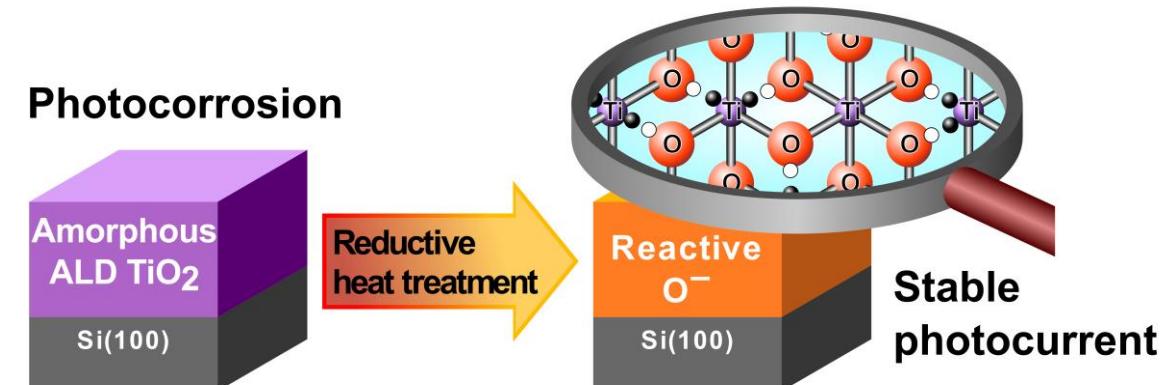


The defect structure of ALD grown amorphous TiO_2 can be modified under oxidative and reductive conditions.

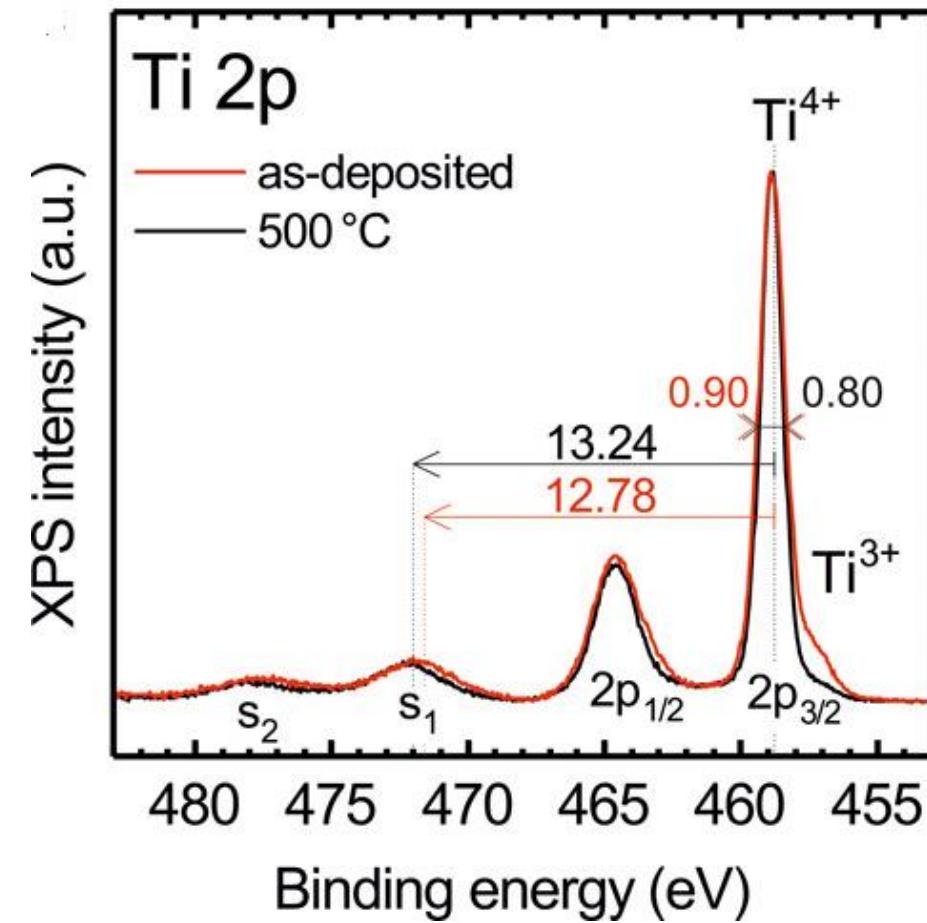
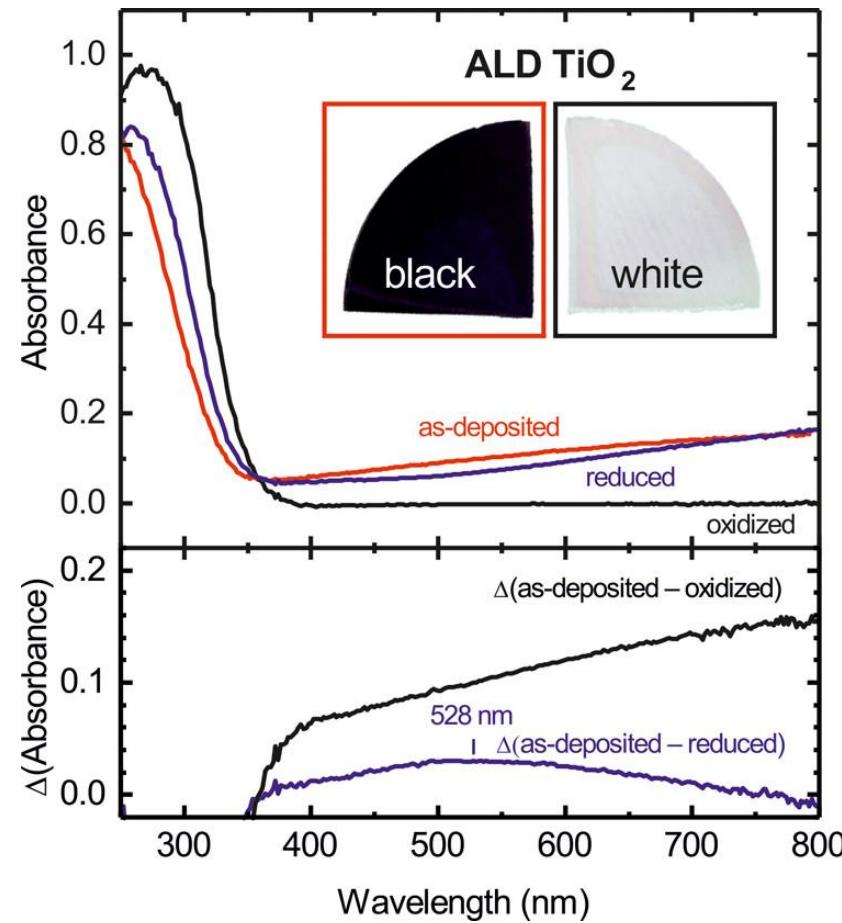
OXIDATIVE HEAT TREATMENT



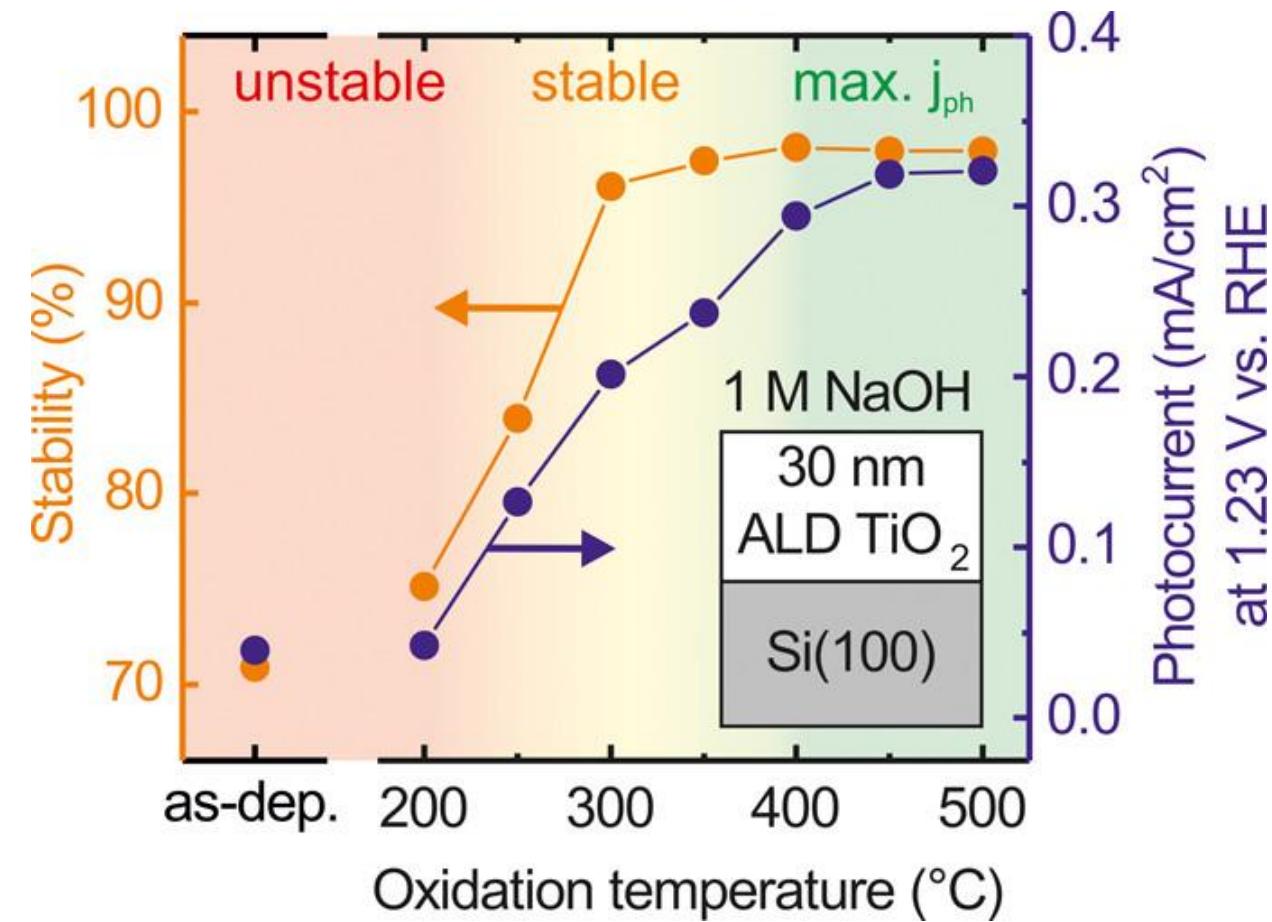
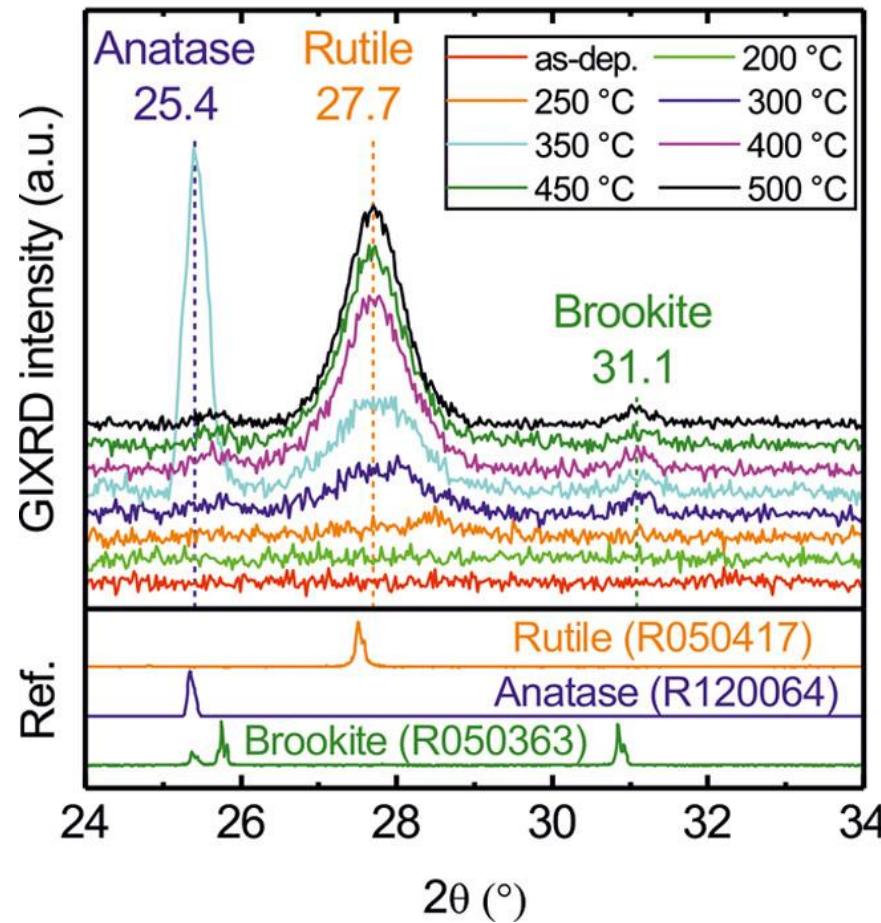
REDUCTIVE HEAT TREATMENT



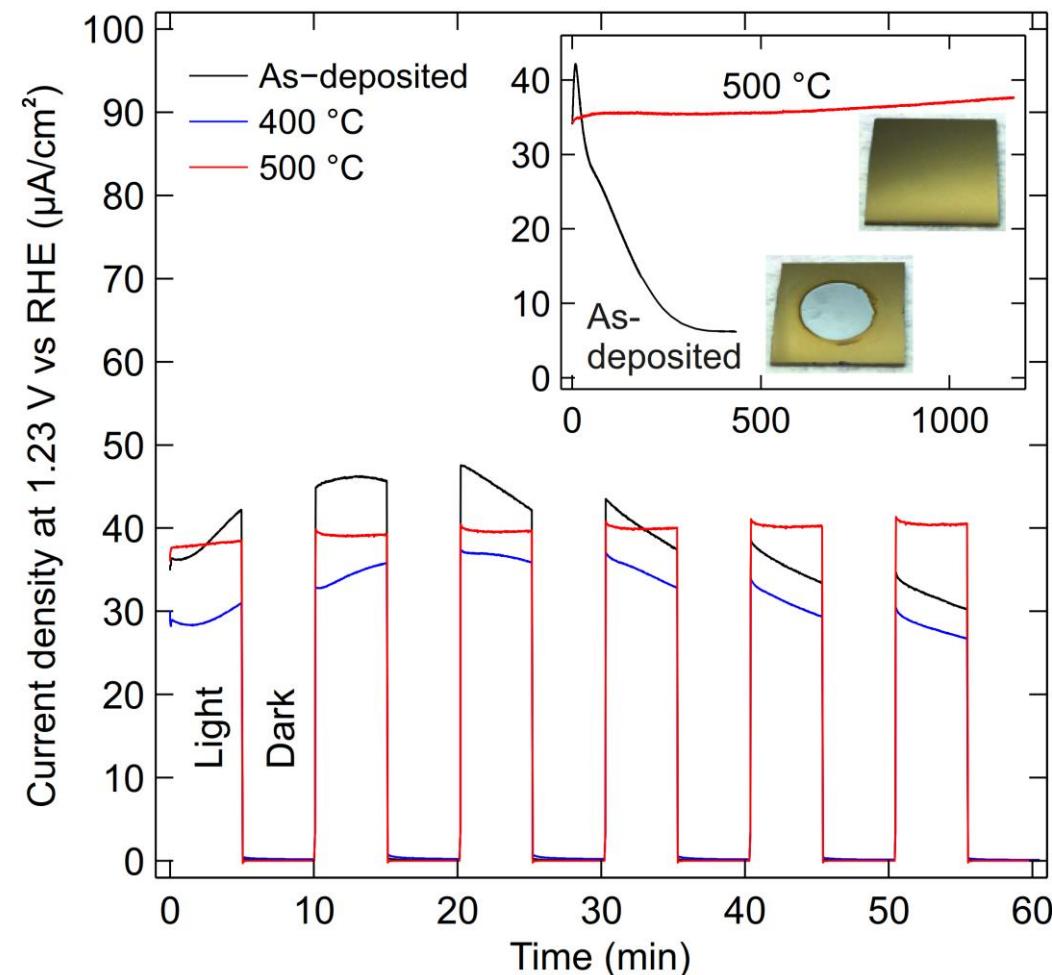
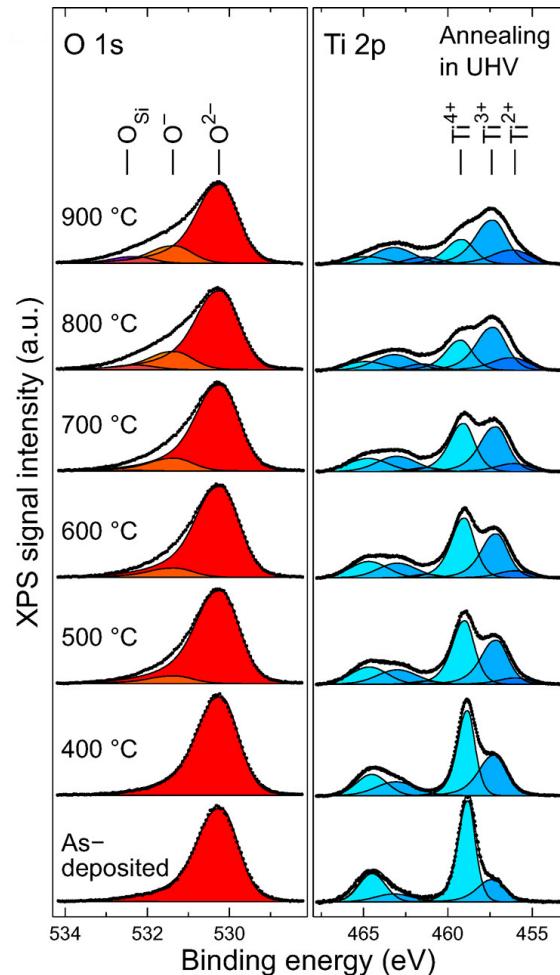
The enhanced absorbance of ALD TiO_2 is due to the Ti^{3+} defects which are oxidized during the heat treatment in air at 500 °C.

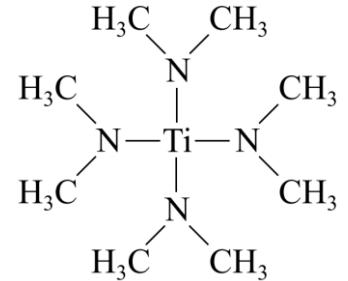


Oxidation at 500 °C results in stable rutile TiO₂ that produces the highest photocurrent for water oxidation.



Reductive heat treatment at 500 °C retains the amorphous phase for TiO₂ but enhances the stability due to the formation of O⁻ species.





Diversity of ALD TiO₂

Sample	Crystallinity	PEC stability	Photocatalytic activity	Color	Conductivity
As-deposited	Amorphous	Unstable	—	Black	"Leaky"
Oxidative heat treatment at 500 °C	Rutile	Good	High	White	Non-conductive
Reductive heat treatment at 500 °C	Amorphous	Good	Medium	Black	"Leaky"

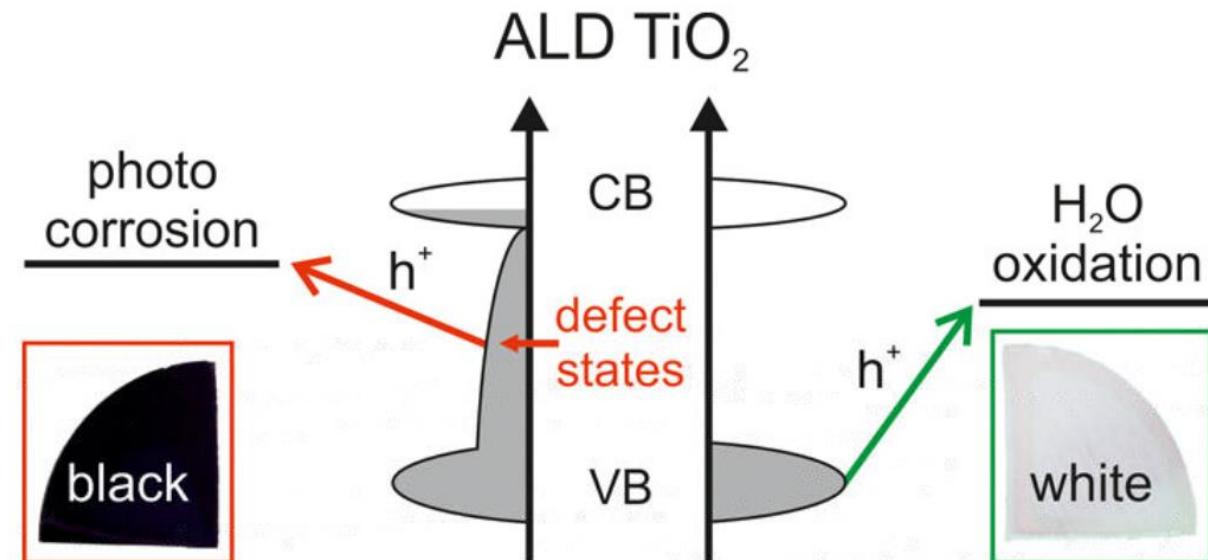
Surface Science

Research group at Tampere University

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Research on the phenomena at surfaces.

The main objectives are to gain insights into the physicochemical surface and interface properties at molecular level and to develop novel materials by functionalizing surfaces on the nanometer scale.

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Diversity of TiO_2 : Controlling the Molecular and Electronic Structure of Atomic-Layer-Deposited Black TiO_2
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References

H. Ali-Löytty, M. Hannula, J. Saari, L. Palmolahti, B.D. Bhuskute, R. Ulkuniemi, T. Nyyssönen, K. Lahtonen, M. Valden, *Diversity of TiO₂: Controlling the molecular and electronic structure of atomic-layer-deposited black TiO₂*, ACS Appl. Mater. Interfaces 11 (3), 2758–2762 (2019). DOI: 10.1021/acsami.8b20608.

M. Hannula, H. Ali-Löytty, K. Lahtonen, E. Sarlin, J. Saari, M. Valden, *Improved stability of ALD grown amorphous TiO₂ photoelectrode coatings by thermally induced oxygen defects*, Chemistry of Materials 30 (4), 1199–1208 (2018). DOI: 10.1021/acs.chemmater.7b02938.