



PSI Center for Neutron and
Muon Sciences

Laboratory for Multiscale Materials Experiments
Paul Scherrer Institut

Public PhD Thesis Presentation

Date: Thursday, May 7, 2026, 13:00h – approx. 13:45h
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Speaker: Kyle Stephens

Design and Characterization of Oxynitride Semiconductor Thin Films for Photoelectrocatalytic Water Splitting

Global energy demands, fueled by growth and digitalization, compel us to develop diverse, low-emission infrastructures. Hydrogen is a key candidate for this mission due to its high energy density and carbon-free combustion. This thesis explores the clean synthesis of hydrogen via photocatalytic water splitting, specifically focusing on semiconducting oxynitrides—materials that balance stability and activity.

To overcome efficiency barriers and enable competitive technology, pulsed laser deposition (PLD) is employed to fabricate thin film photoanodes to investigate fundamental properties and provide improvements. Primary analyses include:

Materials optimization: Novel fabrication of CaTaO_xN_y and $\text{MgTa}_2\text{O}_{6-x}\text{N}_x$ thin films. Optimizing a NiO_x cocatalyst layer to sub-nanometer precision yielded a 15-fold increase in photocurrent.

Characterization tools: The development of a custom operando neutron reflectometry (NR) photoelectrochemical cell to study interfacial phenomena like degradation at the sub-nanometer scale.

Advanced fabrication: Implementation of Pulsed Reactive Crossed-Beam Laser Ablation (PRCLA) using NH_3 , achieving the highest recorded nitrogen content for LaTiO_xN_y films.

Oxynitride fundamentals: Physicochemical analysis of LaTiO_2N powders to understand how structural tilting and nitrogen stoichiometry influence electronic band gaps.

Overall, these findings provide fundamental insights into the oxynitride-cocatalyst-electrolyte interfaces, offering improved catalyst design for industrial-scale water splitting technologies.