ABSTRACT

Nitrides and Oxynitrides as Next-Generation Solar Energy Materials

Nitrides and oxynitrides are emerging classes of materials with a large promise for solar energy conversion due to their high visible-light absorption, tunable electronic structures, and defect tolerance. Although their development has long been hindered by challenging synthesis routes and a tendency toward metastability, recent advances in synthesis and computational modelling are rapidly accelerating progress in the field.

In this talk, I will focus on two nitride semiconductors, $CuTaN_2$ and $ZrTaN_3$, and the structural factors that govern their photoactive properties. In $CuTaN_2$, combined computational and experimental studies reveal strongly anharmonic structural dynamics that lead to an unusual temperature dependence of the bandgap. In $ZrTaN_3$, density functional theory calculations show that the distribution of cations across lattice sites significantly influences the electronic structure and optical response. I will also discuss related oxynitride materials and the role of atomic-scale disorder in tuning optoelectronic properties.

Overall, these results highlight the potential of complex nitrides and oxynitrides as next-generation photoactive materials and demonstrate how atomic-scale structural engineering can be used to tailor their functional properties.

BIOGRAPHY

Dr. Franziska Simone Hegner is currently a Postdoctoral Researcher at the Institute of Chemical Research of Catalonia (ICIQ), where her work focuses on understanding structure-function relationships in complex semiconductor materials for photocatalytic and solar energy applications.

She earned her Ph.D. in Chemical Science and Technology from ICIQ in 2019 under the supervision of Prof. Núria López and Prof. José-Ramón Galán-Mascarós. Following her doctoral studies, she held postdoctoral positions at ICIQ and the Technical University of Munich (TUM), working with Prof. David Egger and Prof. Ian Sharp. Throughout her career, she has built a strong international research profile through collaborations and research stays at leading institutions, including Princeton University, Imperial College London, and the Weizmann Institute of Science.

Her research integrates computational modelling and advanced experimental techniques to unravel the electronic, structural, and dynamical properties of semiconductors and catalytic materials for sustainable energy conversion. In particular, she investigates metal oxides, nitrides, and related materials for photocatalysis and photoelectrochemical water splitting, with the goal of identifying the fundamental descriptors that govern material performance and accelerate the development of efficient technologies for green hydrogen production.

Dr. Hegner has published extensively in leading journals, including *Advanced Energy Materials*, *Angewandte Chemie International Edition*, *ACS Catalysis*, and *The Journal of Physical Chemistry Letters*. Her scientific excellence has been recognized through several highly competitive fellowships, including the Walter Benjamin Fellowship in Germany, the Beatriu de Pinós Postdoctoral Fellowship and the EIGENT Fellowship in Spain for independent researchers.