## Principal Investigators

**Prof. Sanjay Mathur** 

- Chair of Inorganic and Materials Chemistry, Institute of Inorganic Chemistry, University of Cologne. sanjay.mathur@uni-koeln.de



Prof. Ravi Kumar N V Laboratory for High Performance Ceramics, Department of Metallurgical and Materials Engineering, IIT Madras. nvrk@iitm.ac.in



Prof. Silke Christiansen Fraunhofer-Institute for Ceramic Technologies and Systems IKTS; Dept. of Physics, Freie Universität Berlin. schrist1@gwdg.de



## Prof. Hari Kumar K C CALPHAD Laboratory, Department of Metallurgical and Materials Engineering, IIT Madras. kchkumar@iitm.ac.in



Dr. Heechae Choi Junior Group Leader, Institute of Inorganic Chemistry, University of Cologne. h.choi@uni-koeln.de





Scheme for Promotion of Academic and Research Collaboration





Fraunhofer IKTS Tailoring Tantalum Nitrides and Oxy-Nitrides & Designing Electroctalytic Devices for Green Energy

2019 - 2021

## New materials for Green Energy Solutions



## **Project Outline**

With continuing depletion of fossil fuels and natural gases and with ever increasing demand for alternate sources of energy, the current and as well as the next generation will have to seriously work on producing and storing nonpolluting energy forms, referred to as Green Energy. While, in the Indian context, renewable forms of energy based on wind and solar forms are attractive enough and sufficient investments have already been made, other greener forms of affordable energy sources needs to be explored as well.

On the contrary, electrochemical splitting of water for the production of hydrogen which enables conversion of electrical energy to chemical energy and its reversibility is one of the most viable and potential approaches towards "Green Energy". It is imperative to understand that world eventually will make a transition to hydrogen-based economy from a depletable and non-sustainable fossil fuel based economy.

Transition metal nitrides (TMNs) and oxynitrides (free of precious metals such as platinum) have shown immense potential as electrocatalysts and coupled with plasmonic properties these classes of materials are attractive enough to be considered for possible hydrogen evolution reactions. Especially TaN is considered one of the best available TMNs for hydrogen evolution, which catalyses at -0.09V, with activation energies and Tafel reactions close to instant of Cologne Pt(111) at equilibrium that of potential. Apart theoretical studies, the experimental realiis facing zation. several issues that need to be addressed such mechanism as. Simulation for a broader electrochemical window, influence of micro-/nanostructuring, role of plasmonic resonance and role of confinement effect when such nitrides are produced in-situ in a matrix.

Fine-tuning the chemistry, material characterization that includes microscopy and spectroscopy combined with first principle calculations including CALPHAD are vital towards transforming lab-scale research to deployable device-level/reactor-level this fabrication. In research, а highly consisting of interdisciplinary team materials chemists, ceramicists, characterization experts in including correlative spectrotaunnoter scopy coupled with computational materials scientists like would to address these scientific issues at IKTS Characteria U various lenath scales understanding fundamental scientific issues transform lab-scale and research to deployable reactors/devices.

**Total budget** INR 66,000,000 **EUR 85,000** 

**Synthesis** 

Materials

production

**IIT Madras** 

DFT

CALPHAD

Correlative

**Aicroscopy**