The goal of HERON is to combine experimental and computational approaches for an screening of the best suited ionic liquids for their confinement in porous carbons with well defined pore architectures in the full nanopore range. The objective is to identify the best candidates IL-carbon to be tested in the electrochemical reduction of nitrogen to produce ammonia in lab-scale electrochemical reactors in gas/liquid phase. Computational studies allowed to analyze IL with varied cation-anion combinations, to identify the characteristics that define interactions with N₂ molecules. The best candidates identified in the computational screening were tested experimentally to:

1) validate the enhanced adsorption/solubility of N₂ gas in carbon materials with controlled pore characteristics and
2) demonstrate the validity of the approach in the electrochemical Nitrogen Reduction Reaction (NRR).

The novelty of HERON lies in the use of immobilized in a metal-free porous carbon catalyst (as a second component of catalyst) and not as electrolyte.

HERON Results

**Screening of ILs: DFT analysis of N₂-IL interactions; N₂ solubility; electrochemical window**

**Computational screening**

**Experimental Validation**

**Linear Sweep Voltammetry (LSV)** screening of the carbon/IL electrodes in He and N₂ atmosphere

Amount of NH₃ electrogenerated upon chronocoulometry at various potentials and kinetics of the electrocatalytic NRR at -3V

**HERON Outcome and Perspectives**

The electrocatalytic activity of carbon/IL for the reduction of N₂ into NH₃ has been demonstrated. Even though faradaic efficiency and NH₃ production yield still need to be improved, this opens up new perspectives for the electrochemical production of NH₃ from a wide variety of N-sources (e.g., N₂, NOₓ, NO₂) using low-cost carbon electrocatalysts without non-noble metals.

Combined experimental and computational approaches have demonstrated the N₂/carbon/IL interactions as responsible for the increases uptake of N₂ gas inside the nanopores of carbons impregnated with IL.