PROJECTS (2025-)

Keywords: Ligand chemistry, organometallic catalysis, nanocatalysts, hydrogen energy, quantum tunneling, sensors, diamondoids

Project Overview

Our group has a long-term interdisciplinary research program dedicated to the **fundamental and applied development of ligand chemistry for transition-metal reactivity**, spanning homogeneous catalysis, nanocatalysis, sensing, and energy applications. The project exploits **three complementary ligand platforms**—ferrocenyl, diamondoid, and s-aryltetrazine systems—to engineer **robust molecular catalysts, nanoparticle networks, and functional materials** with enhanced cooperativity, selectivity, and durability. A central innovative concept is the **synergistic combination of catalysis with hydrogen quantum mechanical tunneling (HQMT)** to drastically reduce energy barriers in hydrogen transfer reactions.

Main Scientific Axes and Achievements

1. Ferrocenyl Ligands for Advanced Catalysis and Fundamental NMR Theory

- Designed and synthesized **>100 functionalized ferrocenyl ligands**, including robust air- and moisture-stable polydentate phosphines.
- Developed **ultra-low-loading Pd catalysis** (down to 100 ppm) for C–C and C–X (N, O, S, halogen) bond formation with high TONs.
- Introduced pioneering concepts of **through-space scalar spin–spin coupling** in NMR, enabling theoretical separation of through-bond and through-space contributions.
- Ligands commercialized worldwide (HiersoPHOS®, STREM Chemicals).

2. Diamondoid Platforms for Nanocatalysis and Sensing

- Established **bottom-up synthesis of hybrid sp^3-carbon/metal nanomaterials** using rigid diamondoid ligands.
- Demonstrated the **first diamondoid-based gas sensors**, enabling reversible NO_2 (ppb) and NH_3 detection.
- Developed **dense networks of ultrasmall metal nanoparticles** (Ru, Ni, Au) with controlled size, spacing, and cooperative effects for catalysis, plasmonics, and sensing.
- Filed **European patent (2023)** on nanoparticle networks stabilized by polytopic ligands.

3. s-Aryltetrazine Chemistry for Click Reactions and Energy Catalysis

- Invented **Pd- and Cu-catalyzed C–H functionalization strategies** enabling unprecedented derivatization of s-aryltetrazines.
- Developed **orthogonal double click-chemistry platforms** for bioconjugation, photophysics, and materials science.
- Created nitrogen-rich fused heterocycles with novel optoelectronic properties.

Flagship Research Program: Hydrogen Energy & Quantum Tunneling

- Engineered **molecular (Ir, Ru) and nanostructured catalysts** for H_2 release from silanes and boranes.
- Provided experimental and theoretical evidence for **HQMT involvement in catalytic hydrogen activation**.
- Proposed the novel paradigm of **"tunneling-enhanced catalysis"**, combining classical catalysis with quantum effects to reduce energy demand.
- Integrated **AI-assisted nanoparticle design**, advanced microscopy, kinetics, and modeling.

Funding, Outputs, and Impact

- Supported by **ANR, ERC-level projects, IUF, PIA-EUR**, international ANR-DFG collaborations.
- **PhD and postdoctoral supervision**, patents, industrial transfer (SATT maturation), and international collaborations (notably with JLU Giessen).
- Strong impact in **catalysis, energy storage, sensors, and fundamental physical chemistry**.