Initiative
Nouvelles Réactivités
en Chimie Moléculaire
ALLIANCE SORBONNE UNIVERSITÉ

Appel à projets *iDream* 2026

Title of the project:

Dehydrogenation Reaction Networks under Electrochemical Conditions

Acronym : DANDELION

CV of the PIs of each partner

5 significant publications :

- Merging Electrocatalytic Alcohol Oxidation with C-N Bond Formation by Electrifying Metal-Ligand Cooperative Catalysts, S. Kasemthaveechok, P. Gérardo and **N. von Wolff***, *Chem. Sci.,* **2023**, 10.1039/D3SC03408A
- Predicting Ruthenium Catalysed Hydrogenation of Esters using Machine Learning, C. Mishra*, **N. von Wolff***, A. Tripathi, E. Brémond, A. Preiss, N. D. Lawrence and A. Kumar*, *Digital Discovery,* **2023**, 10.1039/D3DD00029J
- Electrification of a Milstein-type Catalyst for Alcohol Reformation, D. Tocqueville, F. Crisanti, J. Guerrero, E. Nubret, M. Robert, D. Milstein **N. von Wolff***, *Chem. Sci.*, **2022**, 10.1039/D2SC04533H
- Prebiotic chemical reactivity in solution with quantum accuracy and microsecond sampling using neural network potentials, Z. Benayad, R. David and **G. Stirnemann***, *PNAS*, **2024**, 10.1073/pnas.2322040121
- Hamiltonian Replica Exchange Augmented with Diffusion-Based Generative Models and Importance Sampling to Assess Biomolecular Conformational

Basins and Barriers, Z. Benayad and **G. Stirnemann***, *J. Chem. Theory Comput.* **2025**, 10.1021/acs.jctc.5c00738

Summary of the project:

DANDELION follows a data-driven strategy to electrify dehydrogenation catalysis for amide bond formation using medium-throughput electrochemistry, quantum calculations and machine-learning. Parallel experiments will provide reproducible datasets across a large parameter spaces. Active learning cycles with fast descriptors including environmental effects will train multivariate ML models, guiding synthesis to desired amide products with high yields.

Support demandé/Project type

Thèse/PhD	X
Post-doc (18 mois)	☐

Reviewers

- Robert Waymouth, Stanford University (Dehydrogenation catalysis): waymouth@stanford.edu
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