

# Emmanuel IKWA

Ph.D Student - IFP Energies Nouvelles  
Rond-point de l'Echangeur, Solaize, France



## FORMATION

### Université Claude Bernard Lyon I

#### ORGANIC CHEMISTRY MASTER'S DEGREE - 2021-2023

- Specialisation in total synthesis, (organometallic) reaction mechanisms, separation and purification of organic products
- Option: theoretical chemistry (Label RCTF in 2023)

## WORK EXPERIENCE

### Ph.D Student - IFPEN (Dept. R061) - From Nov. 2024

#### MECHANISTIC INSIGHTS IN THE CONTEXT OF LOW-CARBON & RENEWABLE HYDROGEN PURIFICATION BY METALLIC CATALYSIS

- Heterogeneous catalysts synthesis & characterisation
- Catalytic tests in gas-solid reactors
- Metallic (Pd & Pt) nanoparticles modelling
- Reactivity of H<sub>2</sub>-O<sub>2</sub> recombination
- Director: Pr D. LOFFREDA
- Supervisors: Drs M. RIVALLAN, T. NARDIN, A. HUGON

### M2 Internship - IFPEN (Dept. R062) - Fev. à Juil. 2023

#### PHENOXY-IMINE TITANIUM-CATALYZED TRIMERIZATION OF ETHYLENE : A THEORETICAL INVESTIGATION

- Theoretical analyses aiming at converging with previous experimental data by mechanistic pathways proposals & experimental perspectives
- Supervisors: Drs. L. MAGNA, K. LARMIER, Pr P-A. PAYARD

### M1 Internship - ITEM (ICBMS) - Janv. à Juil. 2022

#### SALTS EFFECT ON PALLADIUM-COMPLEXES OXIDATIVE ADDITION IN A COMPUTATIONAL STUDY

- Screening salt effects on oxidative addition of methoxybenzene (kinetic and thermodynamic study)
- Supervisors: Dr H. LIANG, Prs P-A PAYARD, M-E PERRIN

## PROFIL

*With a degree in organic chemistry, I am particularly interested in the study of mechanistic aspects of homogeneous or heterogeneous catalytic reactions, with the support of quantum modeling*

## CONTACT DETAILS

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## EXPERTISE

Softwares: Gaussian, Materials Studio, Multiwfn (wavefunction analysis), Pack Adobe, Pack Microsoft, Chemdraw

Codes: Gaussian, VASP

Skills: organic synthesis & purification (RMN, IR, Kofler bench...) ; catalysts preparation (homo- & hetero-geneous) ; reactor resizing

Languages: French & English