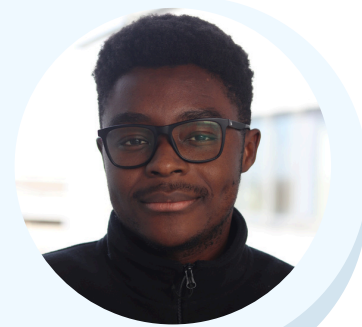


Emmanuel IKWA



Ph.D Student - Looking for a postdoctoral opportunity in heterogeneous catalysis

WORK EXPERIENCE

Ph.D Student - IFPEN & ENS Lyon - Nov. 2023 to Oct. 2026

Mechanistic insights on the H₂-O₂ recombination reaction for renewable H₂ purification (deoxo process) by metallic catalysts

- Catalytic tests in gas-solid reactors (Pt or Pd-based catalysts supported on γ -Al₂O₃)
- Metallic nanoparticles (NPs) modeling with gas phase
- Director & supervisors: Drs D. LOFFREDA, M. RIVALLAN, T. NARDIN, V. SOUCHON, A. HUGON

Two pair-reviewed articles accepted:

- "How Morphological Descriptors Capture the Stability Order in Palladium NPs", *J.Phys.Chem.Lett*
- "Temperature Driven Morphological Changes of Pd NPs from Machine Learning Force Fields", *A.I.Chem*

M2 Intern - IFPEN - Lyon - Feb. to Jul. 2023

Phenoxy-imine titanium-catalyzed trimerization of ethylene: a theoretical investigation

- Supervisors: Drs. L. MAGNA, K. LARMIER, P-A. PAYARD

M1 Intern - ITEM (ICBMS) - Lyon - Jan. to Jul. 2022

Salts effect on palladium-complexes oxidative addition in a computational study

- Supervisors: Drs H. LIANG, P-A. PAYARD, M-E. PERRIN

FORMATION

ENS Lyon

DOCTORAL FORMATION - 2023-2026

Université Claude Bernard Lyon I

ORGANIC CHEMISTRY MASTER'S DEGREE - 2021-2023

- Specialisation in organometallic reaction mechanisms

CHEMISTRY BACHELOR'S DEGREE - 2019-2021

HOBBIES

CHESS - PIANO - SURF - HIKING

PROFILE

Ph. D. in computational chemistry with a solid background in heterogeneous catalysis combining experimental work with theoretical explorations. Developed reactive MLFFs, trying to bridge the gap between realistic molecular view (considering P and T) and macroscopic timescale (approaching the nanosecond)

EXPERTISE

Theoretical skills:

- DFT-based mechanistic pathways
- Active sites definition on nanoparticles
- Molecular dynamics (under relevant pressure and temperature)
- Development of reactive machine learning force fields (MLFFs) trained on-the-fly of DFT calculations

Code: VASP, Gaussian, Python

Experimental skills:

- Catalysts preparation (homo- & heterogeneous) and organic synthesis
- Characterisations of heterogeneous catalysts (HR-STEM, chemisorption techniques)
- Chemical engineering (reactor sizing, mass and heat transfer)

Software: Pack Adobe, Pack Microsoft

Language: French (Fluent) & English (C1-C2)

CONTACT DETAILS

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