

NITheCS Mini-school

Wednesday 11, 18 and 25 May 2022, 14h00 – 15h00

Dr Kingsley Obodo (North-West University) and Dr Cecil Ouma (Next-Einstein forum fellow)

'Quantum ESPRESSO'

ABSTRACT

In this mini-series, we will teach on Quantum ESPRESSO (QE), an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modelling at the nanoscale. It is based on density-functional theory, plane waves and pseudopotentials. QE is a free-to-use code that can be modified for various purposes. This suite of code can be applied to problems in areas including energy storage, drug design, catalysis, materials design and prediction. It is also relevant for researchers in the physical sciences, natural sciences, biological sciences, pharmacology, engineering and other fields.

PRESENTERS



Dr Kingsley Obodo

Dr Obodo is a Computational Scientist in HySA centre of competence at North-West University. His background is in *ab initio* (computational) modelling of various materials, with key interests in the application of physics, materials science, philosophical thinking towards innovations in energy and materials solutions, as well as research, design and development towards sustainability.

Dr Obodo has authored and drafted several technical reports for different projects in addition to numerous publications in peer-review journals. He has over 10 years of experience in research and development, with expertise in scientific programming languages. He plays roles in various projects that have deployed quantitative and qualitative research output, as well as applied these to problems in education, ICT, business and social science among others. He also has several local and international collaborations and is actively engaged in student supervision and mentoring.



Dr Cecil Ouma

Dr Ouma is a Next-Einstein forum fellow and trained computational physicist with over 10 years of experience in *ab initio* studies of material with different applications. He is passionate about STEM and the adoption of Industrial 4.0 in STEM in Africa and developing nations.

He has extensively worked in the field of (renewable) energy as applied to green hydrogen and its associated technologies, specifically in the areas of catalyst and catalytic materials for energy generation, storage and safety applications.

Dr Ouma also has great interests in strategy development and applications, as well as wicked problem solutions using systems thinking and systems dynamics. He has collaboration initiatives with experts in various disciplines.

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