



Faculty of Natural and  
Agricultural Sciences

Fakulteit Natuur- en Landbouwetenskappe  
Lefapha la Disaense tša Tlhago le Temo

# First announcement: SASESMA-2019

Southern African School on Electronic Structure Methods  
and Applications

[www.up.ac.za/physics](http://www.up.ac.za/physics)



There are a large number of electronic structure codes available, but many of the commercial codes are expensive. However, Quantum ESPRESSO is a free, open-source computer code for electronic structure calculations and materials modeling at the nanoscale.

The purpose of the school is to introduce electronic structure theory and related simulation methods, as implemented in the Quantum ESPRESSO package. It will include basic and advanced topics, with an emphasis on computational methods for practical calculations.

The first week of the school will be an introduction to the fundamentals of density functional theory and the associated methods and algorithms, as well as an introduction to Quantum ESPRESSO.

The second week of the workshop will explore the more advanced aspects of Quantum ESPRESSO and will be suitable for advanced postgraduate students and researchers.

The organizing committee of SASESMA encourages researchers and students from research councils, universities and industries to apply by completing the form available at <http://upnet.up.ac.za/sasesma2019>

## Topics:

- Introduction to density functional theory
- Exchange-correlation functionals
- Generation of pseudopotentials
- Ab initio molecular dynamics
- Optical spectroscopies
- Charged defects
- Basic and advance uses of Quantum ESPRESSO
- Access to CHPC

## Invited Speakers:

- Prof N. Chetty, UP, RSA
- Prof E. Lombardi, UNISA, RSA
- Dr Krishna Govender CHPC, RSA
- + 3 international speakers (TBA)

## Organizers:

Chair: Prof Walter Meyer  
[walter.meyer@up.ac.za](mailto:walter.meyer@up.ac.za)

Co-Chair: Dr Edwin Mapasha  
[edwin.mapasha@up.ac.za](mailto:edwin.mapasha@up.ac.za)

**Date:** 10 - 21 June 2019

**Venue:** University of Pretoria  
South Africa

**Contact:** Prof Walter Meyer  
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Dr Edwin Mapasha  
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## Workshop fee:

- Registration fee is R500. Includes light refreshments.
- Participants are responsible for their own accommodation, subsistence and transport.
- Accommodation: There are many hotels and guest houses in the vicinity. Budget options include Airbnb and Backpackers. Please make your own booking.
- Transport: The University is walking distance from the Hatfield Gautrain station and Uber and Taxify are also available.

**Deadline: 15 April 2019**



Make today matter