

# 5th African School on Electronic Structure Methods and Applications (ASESMA - 2018)



**22 October - 2 November 2018**  
**Addis Ababa, Ethiopia**

Further information:  
<http://indico.ictp.it/event/8354/>  
[smr3234@ictp.it](mailto:smr3234@ictp.it)

The School provides an introduction to the theory of electronic structure and other atomistic simulation methods, with an emphasis on the computational methods for practical calculations.

## Directors:

**N. CHETTY**, Univ. Pretoria, South Africa  
**R. MARTIN**, Stanford University, U.S.A  
**S. NARASIMHAN**, JNCASR Bangalore, India  
**S. SCANDOLO**, ICTP, Trieste, Italy  
**N. SERIANI**, ICTP, Trieste, Italy

## Local Organizer:

**T. YOHANNES**, Addis Ababa, Ethiopia

## Description:

The African School series on Electronic Structure Methods and Applications is planned on a biennial basis from 2010 to 2020. Previous schools were held in Cape Town, South Africa (2010), Eldoret, Kenya (2012), Johannesburg, South Africa (2015), and Accra, Ghana (2016).

The School will also cover basic and advanced topics and applications of these methods to the structural, mechanical and optical properties of materials.

The School will include hands-on tutorial sessions based on public license codes (including, but not limited to, the Quantum Espresso package).

During the second week students will be asked to split up in teams and work on specific projects under the guidance of the lecturers and mentors.

## Topics:

- Electronic structure theory;
- Density functional theory and functionals;
- Phonons;
- Magnetism;
- Enhanced sampling methods in molecular dynamics;
- Ab-initio molecular dynamics.
- Optical spectroscopies

## ICTP contacts:

**S. SCANDOLO**, ICTP, Trieste, Italy  
**N. SERIANI**, ICTP, Trieste, Italy

## Invited Speakers:

**O. AKIN-OJO**, ICTP-EAIFR, Rwanda  
**G. AMOLO**, TU Kenya, Nairobi  
**M. CASIDA**, Univ. Grenoble Alpes, Saint-Martin-d'Hères, France  
**M. GATTI**, ETSF, LSI - CNRS, Palaiseau, France  
**G. GEBREYESUS**, University of Ghana  
**E. LUIJTEN**, Northwestern McCormick Sch. of Engineering, Evanston, U.S.A.  
**D. MAGERO**, University of Eldoret, Kenya  
**A. MARINI**, ISM, Rome, Italy  
**R. MAEZONO**, JAIS, Ishikawa, Japan  
**S. NARASIMHAN**, JNCASR Bangalore, India  
**Y. SHAIDU**, SISSA, Trieste, Italy

## How to apply:

Online application:  
<http://indico.ictp.it/event/8354/>

Female scientists are encouraged to apply.

## Grants:

A limited number of grants are available to support the attendance of selected participants, with priority given to participants from developing countries. There is no registration fee.

## Deadline:

**15 July 2018**



The Abdus Salam  
**International Centre  
for Theoretical Physics**  
[www.ictp.it](http://www.ictp.it)  
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