CHPC Forum 27th October 2021

Materials Modeling in Science and Technology

George Amolo and Michael Atambo

http://spas.tukenya.ac.ke

george.amolo@tukenya.ac.ke

General Group Information (MATS862)

- Kenyan group focusing on materials science

- Started at University of Eldoret, later moved to The Technical University of Kenya in 2016

- Goal is on training and mentorship of graduate students and young faculty

- Collaboration, engagement of national, international and other partners is key to our research capacity development

Modeling in Materials Science and Technology:
Themes and National Partner

 Current areas of research are in Physics (Msc and Phd degrees); MSc in Computational Chemistry (lone program nationally)

- Use of high throughput techniques (Aiida – QE and Siesta) for enhanced studies

- Appeals to the Biological Sciences (promise in Bio-informatics) and Engineering

- Kenya Education Network (KENET, also the Kenyan NREN) is a major partner

Current thematic areas and works

Hard Materials

The effects of defects and temperature

Energy Science and Technology

Materials for energy conversion

Complex phenomena

2DEG/2DHG in transition metal oxide interfaces

Other works – Biological Systems and materials for water purification, properties of transition metal oxides

Call for Proposals: Computational Modeling & Materials Science (CMMS) Mini-Grants

kenet
Kenya Education Network

Kenya Education Network (KENET) has one of its mandates as catalyzing collaboration in research and education among member universities and research institutions. KENET promotes collaboration through facilitation of Special Interest Groups (SIGs) in priority academic areas, discovery of active researchers/faculty, and provision of research and education mini-grants to researchers and member institutions, as well as travel grants for faculty and/or graduate students in SIG areas.

Computational Modeling and Materials Science (CMMS) is a special interest group supported by KENET to enhance research capacity development in the use of computational modeling in science and technology. Research work within this group is expected to involve university faculty and graduate students in chemistry, physics and the environmental sciences but strongly welcomes those from other basic and applied sciences. To increase research output directly or by complementing the existing limited work from groups with standard experimental research infrastructure, CMMS has embraced computational modeling which is now considered as an important decision support tool.

CMMS Mini-Grants: Areas of Focus

The research areas of focus for this round of mini-grant funding are:

1. **Materials modeling and development** for energy conversion using basic and applied sciences
2. **Materials science and technology** for environmental safety and health applications

The focus in the *Material Modelling* area is development of knowledge and skills in the area of materials research for energy conversion and related aspects.

The theme in *Materials Science* is open to interests in environmental safety, wellness and mineral formation in solid earth, hence targeting applications in water purification, drug design chemistry, mineralogy and related application aspects.

Mini-Grants Structure

Theme 1 will be awarded 2 mini-grants with theme 2 having 2. A total of four (4) mini-grants will be awarded for the 2018/2019 round of funding. Each mini-grant will be for a maximum of **15,000 USD**. The grant period is 12 months.

Concept Note submission

Concept notes with all supporting documentation should be done through the online submission portal www.kenet.or.ke/call-for-mini-grants-proposals-2018-2019 by **28th February 2019**, 5.00PM EAT.

Eligibility

This call is open to computational modeling and materials science faculty (who are full-time) at any of the KENET member institutions. The lead applicant must be a PhD holder, attained within the last 5 years, and must demonstrate active research interest.

Full Call Document

The full call for proposals document can be accessed/downloaded at

www.kenet.or.ke/sites/default/files/kenet_cmms_mini_grant_call_-_2018_2019.pdf

Kenya Education Network   www.kenet.or.ke   Twitter: @kenet_ke

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East African School on Density Functional Theory and Applications using the Siesta code

siesta

11th – 15th October 2021
Technical University of Kenya
School of Physics and Earth Sciences, Nairobi, Kenya

The school aims at introducing ab initio calculations and molecular dynamics simulation to researchers and postgraduate students of different disciplines, using the SIESTA code.

Description:

Electronic structure codes have become mature enough to be used by scientists not trained in the development of the methods themselves. This is a shift away from traditional practice, in which the know-how and the right to use the code was acquired through a long internship. Nowadays, most codes are distributed with very light licensing restrictions. While this ease of access is in principle a good thing, it carries the risk of uncritical or poor use of the codes by untrained people. There is thus increasing demand for training in the sensible use of these methods, with the goal that the prospective user understands the physical and main technical approximations behind a method. The Siesta code has become quite popular and is increasingly being used by researchers in geosciences, biology, and engineering. Siesta's efficiency stems from the use of strictly localized basis sets and from the implementation of linear-scaling algorithms that can be applied to suitable systems. It's accuracy and cost can be tuned in a wide range, from quick exploratory calculations to highly accurate simulations matching the quality of plane-wave methods. This school aims at introducing the Siesta code to researchers in East Africa. Basic practice, a grounding on the capabilities of the method and the approximations used shall be emphasized.

Topics:

- Basics of density-functional theory, molecular dynamics simulation and geometry relaxation;
- Generation and use of pseudopotentials;
- Construction of basis sets of strictly localized numerical atomic orbitals;
- Localization for linear scaling both in the computation of the matrix elements and in the resolution of the Hamiltonian;
- Influence of the real-space grid and parallelization;
- Post-processing and visualization tools;

Directors:

George AMOLO, Technical University of Kenya, Kenya.
Javier JUNQUERA, Universidad de Cantabria, Spain.
Nicola SERIANI, The Abdus Salam International Centre for Theoretical Physics (ICTP), Italy.
Omololu AKIN-OJO, ICTP-EAIFR, Rwanda.

Local Organizers:

Dickson ANDALA, Multimedia University of Kenya
Michael ATAMBO, The Technical University of Kenya
Victor ODARI, Masinde Muliro University of Science and Technology
James SIFUNA, The Catholic University of Eastern Africa

How to register:

Go to:
https://mrsk.or.ke/news-and-calls/
Enquiries:
siesta2021@tukenya.ac.ke

Grants:

Internet support will be given to selected local participants. There is no registration fee.

Deadline:

24th September 2021

ICTP The Abdus Salam International Centre for Theoretical Physics | IAEA | UC UNIVERSIDAD DE CANTABRIA | TECHNICAL UNIVERSITY OF KENYA

Recent national and regional activities

SIG CMMS Virtual Researchers' Forum – Friday, September 17, 2021
(9.00 AM – 4.00 PM)

Forum Program

Time	Activity	Facilitator / Speaker
9.00 – 9.15 AM	Introductions and Welcome Remarks	Prof. Meoli Kashorda, Executive Director, KENET
9.15 AM – 9.30 AM	Special Interest Groups and Research Engagement at KENET	Prof. Meoli Kashorda, Executive Director, KENET
9.30 AM – 10.30 AM	**Short presentations on the CMMS Projects funded by KENET** 1. Study of photovoltaic absorbers and thermoelectric materials using density functional theory – *Dr. George Manyali, Kaimosi Friends University College* 2. Density Functional Theory investigation of possible Fe2 P-type materials for near-room temperature refrigeration. – *Dr. Winfred Mulwa, Egerton University* 3. Modeling and Additive Manufacturing of Frontier Materials for Electrochemical Energy Conversion and Storage Systems – *Dr. James Mutua, Jomo Kenyatta University of Agriculture and Technology* 4. Computer-aided design and development of porphyrin-based photosensitizers for Water purification - *Dr. Holiness Nose, Technical University of Kenya* 5. Building of Heavy Metal Cations -Binding of Heavy Metal Cations - Ethylenediamine (Modified) Maize Tassel Complexes: Insights from the Density Functional Theory – Molecular Dynamics (DFT-MD) Simulations – *Dr. Lucy Kiruri, Kenyatta University*	Prof. George Amolo, Research Associate, KENET
10.30 – 10.45 AM	**Virtual Health Break**	
10.45 AM – 11.45 AM	**Panel Discussion** – International Partnerships in Materials Science Research and Access to Computational Resources	Prof. George Amolo, Research Associate, KENET

Time	Activity	Facilitator / Speaker
	1. *– Prof Dickson Andala Materials Research Society of Kenya* 2. *– Dr Akin-Ojo Omololu Director – ICTP Africa, Africa Campus* 3. *– Prof Sara Bonella – Deputy Director-CECAM* 4. *– Dr. Ciira Maina, Data Science Africa and Center for AI research, DKUT*	
11.45 AM – 12.30 PM	KENET and Partners Computational Resources and Software Appliances for Researchers and Faculty	Ronald Osure, Software Development Lead, KENET
12.30 PM – 2.00 PM	**Virtual Lunch Break**	
2.00 PM – 2.45 PM	**Plenary discussion** on the Priority Research Areas in CMMS for FY 2021-2022 Call for CMMS Research Grant Proposals	Prof George Amolo, Technical University of Kenya and Research Associate KENET
2.45 – 3.00 PM	Vote of Thanks and Closing Remarks	Mr. Kennedy Aseda, Chief Technology Officer, KENET

https://events.kenet.or.ke/event/33/ – registration shall remain open up to September 16, 2021>

Recent national and regional activities

Current and recently graduate students

Phd

James Sifuna, Geoffrey Arusei and Glady King'ori

Carolyn Bakasa.

MSc

Perpetua Muchiri, Bill Oyomo, Samson Gurema

Renson Mayunga.

Recent graduates

Phd - Dr Victor Meng'wa, Dr Miriam Chepkoech

Dr Fred Omboga.

MSc – Lynet Allan

Acknowledgments

- KENET and ICTP
  International Collaborators
   Cecil Ouma, HySA, South Africa
   Javier Junqera, Spain
   Nicola Seriani, (ICTP), Trieste, Italy
   Daniel Joubert, Wits, South Africa

 Local Collaborators
   Holliness Nose – Technical University of Kenya
   Nicholas Makau – University of Eldoret
   Korir Kiptiemoi – Moi University
   George Manyali - KAFUCO