COMPUTATIONAL MATERIALS SCIENCE GROUP

DEPARTMENT OF PHYSICS

RESEARCH AND SCHOLARLY ACTIVITIES

2008 – 2012

Introduction

The Computational Materials Science Group (CMSG) focuses on problems dealing with modeling aspects that support experimental Solid State Physics, Materials Science, Genomics, among other multidisciplinary scientific aspects. Interested staff and students from University of Eldoret, other universities and tertiary institutions in Kenya and the region are invited to undertake collaborative work with us. We have several international collaborative links ensuring that our research themes produce high quality peer-reviewed international publications and have current relevance to community. This report presents highlights of some of the group activities from 2008 - 2012. The group currently consists of the following members:

Staff Members

1. Nicholas W Makau, BSc (Moi) MSc (Moi) PhD (Witwatersrand, RSA)
2. George O Amolo, BSc (Moi) MSc (Nairobi) PhD (Witwatersrand, RSA)
3. Joseph Z Mapelu, BSc (Moi) MSc (Nairobi) PhD (Moi, Kenya)
4. Rogers Koech, BSc (Moi) (MSc candidate-JKUAT)–Computer Science- (System Administrator)

Current Postgraduate Students

1. Winfred Mulwa, BSc (Kampala) (MSc - Eldoret)
2. Henry Otunga, BSc (Maseno) MSc (Maseno) (Dphil candidate - Maseno/Eldoret)
3. Phillip W O Nyawere, B.Ed (Sc) (Kenyatta) MSc (Moi) (PhD candidate-Eldoret/ICTP)
4. Dennis Magero, BSc (Moi) – Chemistry (MSc candidate - Eldoret)
5. Mike Atambo, BSc (Moi) – Physics (MSc candidate - Eldoret)
6. Victor Meng'wa, BEd Sc (Egerton) (MSc candidate – Eldoret)
7. Patrick Mwonga, BEd Sc (Kenyatta) (MSc candidate – Eldoret)
8. Peter Kirui, BEd Sc (Egerton) (MSc candidate – Eldoret)

Peer-Reviewed Publications

C N M Ouma, M Z Mapelu, N W Makau, G O Amolo and Ryo Maezono, *Quantum Monte Carlo Study of Pressure-induced B3-B1 Phase in GaAs*, Phys. Rev. B86, 104115 (2012).

I T Motochi, N W Makau and G O Amolo, Metal-Semiconductor Ohmic Contacts: *An ab initio Density Functional Theory Study of the Structural and Electronic Properties of Metal-Diamond (111)-(1×1) Interfaces;* Diamond and Related Materials, vol 23 (2012) 10 – 17.

K K Korir, G O Amolo, N W Makau and D P Joubert, *First Principle Calculations of the Bulk Properties of Group 4d Transition Metals*, Diamond and Related Materials, 20, 157 (2011).

T. E. Derry, N. W. Makau, and C. Stampfl, *Oxygen Adsorption on the (1 × 1) and (2 × 1) reconstructed C (111) Surfaces: a Density Functional Theory Study*, J. Phys.: Conden. Matter, 22 p. 265007 (2010).

C. Stampfl, T.E. Derry and N.W. Makau, *Interaction of diamond (111)-(1x1) and (2x1) surfaces with OH: A first principles study*, . Phys.: Conden. Matter., **22**, 475005 (2010).

G.O. Amolo, J.D. Comins, R.M. Erasmus, T.E. Derry, *Studies of Defects in Photonic Materials*, Physica B: Condensed Matter, vol 404, Issue 22, 4370 (2009).

J. D. Comins, G. O. Amolo, T. E. Derry, S. H. Connell, R. M. Erasmus, M. J. Witcomb, *Ion beam induced defects in solids studied by optical techniques*, Nuclear Instruments and Methods in Physics Research B, vol 267, 2690 (2009).

T.E.Derry, N.W.Makau and Nic Van der Berg, *Diamond Surfaces polished both mechanically and manually: an atomic force microscopy study (AFM),* Diamond and Related Materials, 15 (2008), 160-163.

Conferences Presentations

Dennis Magero, Victor Meng'wa and Winfred Mulwa made conference presentation in the 1st Materials Science and Nanotechnology Conference held in Kenyatta University in August 2012. The works they presented are, respectively, *(1) The Hydrogen Economy – Materials for Hydrogen Storage Surface; (2) Calculations for (110) Rutile TiO_2 and SnO_2 for Dye Sensitized Solar Cells* and *(3) First Principle Calculations of $Nb:TiO_2$ for Solar Cells Applications*.

George Amolo attended a workshop on Solar Energy Materials in Trieste, Italy and made a presentation: *First Principle Calculations of bulk TiO_2 and its suitability for Solar Cell Applications on doping with selected impurities,* 2011.

K K Korir**,** G O Amolo**,** N W Makau and D P Joubert, *First Principle Calculations of the Bulk Properties of Group 4d Transition Metals,, 5th Moi University International Conference* 3 – 7th August 2009, Eldoret, Kenya.

I Motochi**,** N W Makau and G O Amolo, *Surface Calculation Studies of Metal Atoms on Diamond, 5th Moi University International Conference,* 3 – 7th August 2009, Eldoret, Kenya.

G S Manyali**,** G O Amolo and N W Makau, *Magnetic Properties of group 3d Transition Metals, 5th Moi University International Conference*, 3 – 7th August 2009, Eldoret, Kenya.

G O Amolo, N W Makau, K K Korir, I Motochi and D P Joubert, *Opportunities in Computational Materials Science Modeling in Eastern and Southern Africa, 1st Conference of the Materials Science and Solar Energy in Eastern and Southern Africa*, 13 – 15th October 2009, University of Dar es Salaam, Tanzania.

G O Amolo, J D Comins and T E Derry, *Effects of Irradiation on the Optical Properties of Tin-Doped Indium Oxide Thin Films, 1st Regional Conference of the Materials Science and Solar Energy in Eastern and Southern Africa*, 13 – 15th October 2009, University of Dar es Salaam, Tanzania.

Research Funding Attracted by the Group

TWAS funding to extend the computer cluster size, USD 11,000 (11-212RG/PHYS/AF/AC_1-UNESCO FR: 3240262670) (2012)

Awarded a STI grant (Ksh 6 Million – NCST/5/003/4th STI CALL/050) from the National Council of Science and Technology, Government of Kenya, to work on Materials for Solar Energy Applications (October 2011).

Awarded by the Republic of South Africa Government R 91,290 under the African Laser Centre, Pretoria (December 2009) for Laser-Matter Interactions Research in collaboration with Dr. Andrew Forbes, National Laser Centre, Pretoria, RSA.

Awarded a STI grant (Ksh 2.34 Million – NCST/5/003/0241) from the National Council of Science and Technology, Government of Kenya, to build a Computational Material Sciences Laboratory (July 2009).

Awarded by the Republic of South Africa Government R 167,620 under the African Laser Centre, Pretoria (May 2009) for Laser-Matter Interactions Research in collaboration with Dr. Andrew Forbes, National Laser Centre, Pretoria, RSA.

Received from the Moi University Research Fund – MU/DVC/REP/27C (Ksh 110,000) to build a Computational Material Sciences Laboratory (October 2008).

Research/Training Visits

2012

1. George Amolo made a 3 month visit in May to the ICTP under the Associateship program.

2. Phillip Nyawere made his fourth STEP ICTP/Moi University PhD sandwich visit to the ICTP on 31st June 2012 for 6months. Host: Prof Sandro Scandolo.

2011

1. Phillip Nyawere made his third STEP ICTP/Moi University PhD sandwich visit to the ICTP on 31st June 2011 for 6 months. Host: Prof Sandro Scandolo.

2010

1. Rogers Koech and Edmund Ochieng – were invited to participate in Cluster Administration training in Addis Ababa, Ethiopia in August 2010 – University of Addis Ababa with full funding from the ICTP.

2. Phillip Nyawere made his second STEP ICTP/Moi University PhD sandwich visit to the ICTP on 31st June 2011 for 6 months. Host: Prof Sandro Scandolo.

3. R Rop made his second visit to the National Laser Centre (NLC), Pretoria (South Africa) on the May 2010 for a period of 6 months. Travel and living expenses were paid by the NLC and the African Network of Scientific and Technology Institutions (ANSTI). Host: Dr Andrew Forbes.

4. Emily Ouma made a visit to the National Laser Centre (NLC), Pretoria (South Africa) on the May 2010 for a period of 2 and half months. Travel and living expenses were paid by the NLC

5. Nicholas Makau made a collaborative visit to the National Laser Centre, Pretoria (South Africa) in September 2010 for 6 days. Travel and living expenses were paid by the NLC. Host: Dr Andrew Forbes.

6. George Amolo made a 3 month visit in May to the ICTP under the Associateship program.

7. George Manyali, Korir Kiptiemoi, Isaac Motochi, Phillip Nyawere, Cecil Ouma and Nicholas Makau attended the 2nd African School on Electronic Structure Methods and Applications (ASESMA) School in July 2010 held in Cape Town, South Africa. They were fully sponsored by the International Centre for Theoretical Physics (ICTP).

8. Rogers Koech, Edmund Ochieng, Cecil Ouma and George Manyali visited the Centre for High Performance Computing, Cape Town, South Africa. The first three named persons were sponsored by the ICTP while the fourth one was sponsored by the International Business Machines (IBM).

2009

1. R Koech – was invited to participate in the installation of a Geosciences computer Cluster in Addis Ababa, Ethiopia in October 2009 – University of Addis Ababa with full funding from the ICTP.

2. R Koech – was invited to attend a School on High Performance and Grid Computing – International Centre for Theoretical Physics – 30th November - 12th December 2009. Travel and living expenses were paid in full by the ICTP.

3. P W O Nyawere made his first STEP ICTP/Moi University PhD sandwich visit to the ICTP on 20th June 2009 for 6 months. Host: Prof Sandro Scandolo.

4. R Rop made his first visit to the National Laser Centre (NCL), Pretoria (South Africa) on the 10th August 2009 for a period of 3 months. Travel and living expenses were paid by the NLC and the African Network of Scientific and Technology Institutions (ANSTI). Host: Dr Andrew Forbes.

5. G O Amolo made a collaborative visit to the National Laser Centre, Pretoria (South Africa) on the 3rd of September 2009 for 10 days. Travel and living expenses were paid by the NLC. Host: Dr Andrew Forbes.

2008

1. Korir Kiptiemoi and George Amolo attended the 1st African School on Electronic Structure Methods and Applications in Cape Town, South Africa, from the 14th – 31st of July 2008. School was sponsored fully by ICTP and National Research Foundation, Republic of South Africa.

2. Isaac Motochi, Nicholas Makau and George Amolo attended the East African School on Electronic Structure Methods in Addis Ababa, Ethiopia, from 15 – 26th September 2008. School was fully sponsored by ICTP and University of Addis Ababa.

3. George Amolo attended a workshop on Radiation Effects in Materials, Trieste, Italy, from 18 – 24th November 2008. Partial travel and full living expenses were met by ICTP

2012- Visitors

1. Dr Ryo Maezono and Dr. Kenta Hongo of the Japanese Advanced Institute of Science and Technology (JAIST) visited our group in February 2012. Dr Maezono and Dr. Hongo are experienced users of Quantum Monte Carlo and are currently guiding a graduate student (MSc), Mike Atambo, to use the CASINO code. They have both given a seminar entitled 'Electronic Structure Calculation using Monte Carlo Methods'

2011- Visitors

1. Dr Ryo Maezono and Dr. Kenta Hongo and Kentaro Hayashi of the Japanese Advanced Institute of Science and Technology (JAIST) visited our group in March 2011. Dr Maezono and Dr. Hongo are experienced users of Quantum Monte Carlo and are currently guiding a graduate student (MSc), Mike Atambo, to use the CASINO code. They gave s seminar on 'Quantum Monte Carlo Methods' and also demonstrated how to build a computer cluster.

2010- Visitors

1. Dr Ryo Maezono of the Japanese Advanced Institute of Science and Technology (JAIST) visited our group in April 2010. Dr Maezono is an experienced user of Quantum Monte Carlo and is currently guiding a graduate student (MSc), Cecil Ouma, to use the CASINO code. He gave a seminar entitled 'Electronic Structure Calculation using Monte Carlo Methods'
2. Professor Andrew Forbes of the National Laser Centre (NLC, Pretoria, South Africa) visited our group in May 2010. Prof Forbes is the Chief Researcher at the NLC and an adviser to the State Minister of Science and Technology on Laser Research and Technology related matters. He guided our graduate students, Ronald Rop (PhD) and Emily Ouma (MSc). Prof Forbes presented a seminar entitled 'Introduction to Lasers'
3. Dr. Nina Dudnik from the Seeding Laboratories (USA) made a visit to our computer laboratory in May 2010.
4. The National Council of Science and Technology, Kenya Government, monitoring and evaluation team visited our group in April 2010.
5. Ms Emily Aradi, a group member and currently a Phd student at the University of the Witwatersrand, South Africa, gave a seminar entitled 'Modifications of Soft Hexagonal Boron Nitride to Ultrahard Cubic Boron Nitride by Ion Implantation'.

Local and International Collaborators

1. Local

(a) Robert Gateru – Kenya Methodist University: Area of Experimental Device Physics

(b) Christoper Maghanga – Kabarak University: Area of Solar Energy Energy Materials

(c) Robinson Musembi and Julius Mwabora – University of Nairobi: Area of Solar Energy Materials

2. International

(a) Ryo Maezono and Kenta Hongo – Japan Advanced Institute of Science and Technology (JAIST), Ishikawa, Japan: Area of Computational Materials Science

(b) Daniel Joubert - University of the Witwatersrand (Wits), Johannesburg, South Africa: Area of Computational Materials Science

(c) Sandro Scandolo - International Centre for Theoretical Physics (ICTP), Trieste, Italy: Area of Computational Materials Science

(d) Mark Casida – University of Grenoble, Paris, France: Area of Computational Quantum Chemistry.

(e) Andrew Forbes – National Laser Centre, Pretoria, South Africa: Area of Laser Physics

Mentorship Program in Physics and a Multidisciplinary Approach to Scientific Problem Solving using Computational Sciences

Computational Materials Science Group
Department of Physics
Chepkoilel University College
(A Constituent College of Moi University)

Eldoret, Kenya

January 2012

Introduction

The role of science and technology in sustainable development is clearly evident in the economies and the quality of life of citizens in the developed world. Some of the outstanding factors in this regard are related to the skilled manpower produced by their Research Institutions and Universities as well as their ability to convert scientific results into consumer end products. There is direct evidence of a link between development and investment in scientific research [1].

In the last decade, computer technology has greatly influenced the direction of research and in specific cases empowered companies through efficient automation of production, and even the ability to test and evaluate models before implementation and utilization. This has consequences of cutting costs quite significantly. The physical sciences, in particular Physics, have several aspects that deal with modeling of natural and artificial systems that have relevance in the current consumer driven markets and research institutions. Associated students have the potential to be very productive if sufficiently trained to be able to work in an environment where a multidisciplinary approach to scientific problem solving is emphasized.

The following points are identified as issues that have lagged behind in the current evolution of science in the developing world:

1. The current trend of the use of Information communication technology (ICT) in many areas of the economy has not been matched with adequate high end training and skills to enable optimum use of the technology and consequently benefits to the consumer and the country as a whole.

2. The number of Physics students has decreased over the years due to perceptions that they do not automatically fit into the traditionally professional jobs.
3. The effectiveness of the teaching of Physics has not improved significantly at all levels over the years.
4. The utilization of Physics graduates in industries and research institutions is still limited.
5. Gender disparity in Physics enrollment in the Universities and tertiary institutions remains very noticeable.

It is noted that tertiary institutions in this country have not substantially modified their curricula to focus on skills and expertise that would make Physics students appreciate the subject and also be readily employable in the local and international job market.

It is also clear that many of these institutions have not sufficiently embraced a cross-discipline mode of training that may be vital to the needs of industry. The goal of this program will therefore be the mainstreaming of Physics in the national development process. The enhanced plan to develop a program that will encourage a cross-discipline approach to training of students with a strong bias to the use of computational sciences thus seems very appropriate. There are initiatives by institutions of global reputation such as the International Centre for Theoretical Physics (Italy, Trieste) that are making serious attempts to find common working relations between Physics and Biology by organizing joint workshops (ICTP - SMR2336 – April 2012) emphasizing this need for cross-discipline work that may prove to be beneficial in areas such as food security and health, among other fields, which are crucial to the developing world. The Government of Kenya has also produced an economic growth blue print, Vision 2030, that needs well trained and sufficient manpower to realize this Vision.

The Computational Materials Science Group (CMSG) has been running a mentorship program since 2007 (see attached Table 1). In this program sufficiently meritorius and self-driven 4th year BSc (Physics) students are invited to spend time with the group after their final year for a period of 3 months during which they are assigned projects to undertake. Efforts are made to attract female students and as seen in table 1 where two female students have successfully gone through this programme. In the initial stages, staff members in the research group used personal funds to pay for the accomodation and upkeep of the students. However, between 2009-2011, the mentorship program students were funded from the National Council for Science and Technology, Government of Kenya (NCST) grant awarded

to the group. In addition to other roles assigned to them, they also assisted with setting up the Chepkoilel Computer cluster that was also funded by the NCST. It is worthy noting that if the cluster was set up by personel hired from the private sector, it would have cost the research group an estimated Ksh 300,000 (approximately Euros 3000 at the current exchange rate – 1Euro to Ksh 100) which is 10 times what it costs by hiring the students. As a shift from the past when only BSc (Physics) students were considered, a BSc Computer Science student was also invited to the mentorship program in 2010 to assist with the setting up of the computer clusters. Table 1 shows details of students who have gone through the mentorship program and their current status:

Table 1: Past and present mentorship students of the CMSG since 2007

Period (Academic Year)	Student Name	Intermediate Training after BSc	Current Student Status
2007/08	Nyibule, Sheth BSc (Physics) nyakwarkabasa@yahoo.com	Basic Dip, Dip; ICTP, Italy	PhD, Rochester, USA
2008/09	Aradi, Emily BSc (Physics) Emily.Aradi@students.wits.ac.za	MSc – Wits, South Africa	PhD - Wits, South Africa
2009/10	Ouma, Cecil BSc (Physics) moronaptaly84@gmail.com	MSc – Chepkoilel University College	PhD- Pretoria, South Africa
2010/11	Mutisya, Sylvia BSc (Physics) mueni_sylvia@yahoo.com Ochieng, Edmund BSc (Comp. Science) ochienged@gmail.com	MSc – Chepkoilel University College Intern system admin-CMSG	ICTP basic diploma, Diploma, Trieste, Italy Level 2 Linux Administrator, Rackspace Hosting Texas, USA
2011/2012	Atambo, Mike BSc (Physics) mikeat4999@gmail.com	MSc – Chepkoilel University College	MSc – thesis submitted for examination
2012/2013	Buko, BSc (Physics) Elkana, Samson and the others		

Well designed scientific mentorship programmes may be considered as an equivalent of the business incubation models that have recently been regarded as a blue print for successful entry into entrepreneurship. In this light, students will be mentored through carefully chosen projects in materials science and other topical cross-cutting themes that will be geared towards achieving the best results for them and their future endeavors, in line with the goal of this program, the mission statement of Chepkoilel University College and the country's vision for economic growth, Vision 2030 [2, 3]. To maintain and encourage the students in this program, financial and other forms of support will be provided for suitable periods during the long vacations and other arranged times.

Objectives

I. Increase the number of Physics students with above average competence in computer skills such as modeling and open source systems in the period 2012 – 2014 and encourage them to join graduate studies.
II. To attract 2-3 Kenyan citizens, yearly, in the diaspora with PhDs in basic science, who are willing to come home to join tertiary and research institutions as a stop gap towards joining academic departments in Kenyan Universities in the period 2012 – 2014.
III. Improve the number of science graduate students with cross-cutting scientific knowledge in the period 2012-2014.

Selection Criteria and the Mentorship Approach

I. Undergraduate students with top grades as well as sufficient motivation and self-drive are selected to participate in the mentorship programme. The selection is usually done by the academic staff members of the group.
II. Postgraduate and postdoctoral students with good academic standing as well as publications in peer-reviewed journals will from this year, 2012, be expected to write applications to the group outlining reasons and providing motivation to be considered to participate in the mentorship /postdoc programme.

Selection Process and Activities:

1. Advertisement,
2. Recruitment of Students ,

3. Assignment of projects and mentors,
4. Carry out research,
5. Presentation of report and appraisals as well as possible publications of results.

Justification For Request for Funding

University of Eldoret has limited funds that are channeled towards other critical areas. However, the University provides the students with laboratory space and pays for electricity as well as other basic amenities.

Expected Output

I. The undergraduate students undergoing the mentorship program will be required to produce a report of their projects and in outstanding situations publications. Where possible, the students will be sponsored to local attend scientific meetings. The students will also be requested to provide appraisals of the program.

II. Postdoctoral students will be expected to produce peer-reviewed articles as well as guide the undergraduate and postgraduate students of the group.

Proposed Budgetary Estimates

Table 2: Estimated Undergraduate Mentorship Costs - 2012 – 2014

Cost per student for accommodation and upkeep per month	Proposed number of students per year	Months per year	Number of years	Total Cost
Ksh 11,000	5	3	3	Ksh 495,000 (Euros 4950) (1 Euro: Ksh100)

Table 3: Estimated Postdoctoral Mentorship Costs - 2012 – 2014

Cost per student for accommodation	Proposed number of students per year	Months per year	Number of years	Total Cost

and upkeep per month				
Ksh 30,000	2	12	2	Ksh 1,440,000 (Euros 14,400) (1 Euro: Ksh100)

Follow-Up Activities

Annual meetings of former mentorship students for scientific activities in the form of seminars and exchange of experiences with staff members and the current postgraduate students will be arranged. Already, the CMSG planned for first activity and held a series of seminars on the 5th of January 2012. The Deputy Principal – Academic and Student Affairs officially opened the first series (See attached photo of participants below, which includes Ag. DVC-APF and Ag. DVC-ASA).

References

[1] Unesco, www.unesco.org/science/editorial , visited on the 29th March 2007.

[2] Vision 2030 – http://www.vision2030.go.ke/: Jan 2012

[3] Strategic Plan, National Council for Science and Technology, www.ncst.go.ke: Jan 2012

Facilities

1. Linux PC's with secure shell capabilities to connect remotely to sites of our collaborators clusters namely:
   a) Prof. Daniel Joubert, School of Physics, University of the Witwatersrand, South Africa (using VASP).
   b) Dr Ryo Maezono, Japanese Advanced Institute of Science and Technology (QMC and Quantum Espresso)
2. Computer laboratory with Linux PC's installed with DFT codes – Quantum Espresso, Castep, Open source QMC – Casino.
3. 3 i7 PC cluster.
4. Local Sun-Server 52 core cluster funded by the Government of Kenya.

Hosting of National and International Schools/Workshops

The CMSG in conjunction with the Department of Physics, University of Eldoret, hosted various national and international schools/workshops as outlined in the following sections, with the aim of supporting physics training in the country. These have a had a significant impact in the sense that there has been a renewed interest in physics by more undergraduate students inquiring to join various graduate degree training programs both locally and internationally. Similarly, there has also been renewed interest in postgraduate studies.

National Physics Forum
Chepkoilel University College
9 -10th February

The Forum was held on 9th and 10th February at Chepkoilel University College in Eldoret and was officially opened by the Principal of Chepkoilel University College, Prof. Elijah Biamah. Its main theme was "Mainstreaming Physics in National Development and Kenya Vision 2030". It was attended by 21 Physicists from academia and industry (KEBS). Its specific objectives were:

1. To interrogate on how to revive the activities of the Kenya Physical Society.
2. To come up with modalities of engaging government in its implementation of Kenya Vision 2030.
3. To brainstorm on the current state of Physics in the country and how to get involved in making a positive change.

See national physics forum photo below, which includes the Ag. Vice Chancellor.

Sponsors: National Council for Science and Technology (Now the National Commission for Science, Technology and Innovation) and Chepkoilel University College (Now University of Eldoret).

ASESMA 2012
The Second African School of Electronic Structure Methods and Applications (ASESMA), Chepkoilel University College, Eldoret, Kenya
28 May – 8 June, 2012

Summary

ASESMA 2012, the second school in the biennial series, fulfilled crucial goals: It was the first held outside South Africa and its success was an essential step in the goal of trans-African collaborative network. This school demonstrated the progress toward self-sustaining infrastructure with participants from the 2010 school doing more advanced work and tutoring new students. These students have been in communication among themselves as well as with lecturers and mentors since 2010. Many have had opportunities for study, international collaborations, and meetings in Europe. The successful mentor program continued and extended by the tutors. All this led to an air of optimism this year.

The program at the 2012 school continued the development of theoretical and computational studies of real material systems, with lectures, discussions, hands-on computation and projects. This year the topic was energy. In addition to basic lectures on theory and methods, there were lectures on catalysis, optical properties, and splitting of water at interfaces for solar energy. Each student was involved in a project the second week: hydrogen evolution on metals such as Pt, optical properties of FeS_2, or electronic properties of graphene and boronitrene.

After the school, some participants plan to continue with projects started at ASESMA 2012 while others plan to proceed with studies and international collaborations made possible by contacts at the school. Others still have initiated international collaborations, and some others will attend meetings in Europe, Africa and Japan. Participants from the Congo and Cameroon are planning a joint regional network.

Leaders and Participants

Directors: George Amolo and Nicholas Makau (Chepkoilel University College, Eldoret, Kenya), Nithaya Chetty (University of Pretoria, South Africa), Richard Martin (University of Illinois, USA), and Sandro Scandolo (International Centre for Theoretical Physics, Trieste, Italy)
Lecturers: Thomas Bligaard, Roberto Car, Mark Casida, Ralph Gebauer, Stefano de Gironcoli, Paolo Giannozzi, Daniel Joubert, Lev Kantorovitch, Bernard M'Passi-Mabiala, Ryo Maezono. Shobhana Narasimhan, Annabella Selloni, Renata Wentzcovich
Mentors: Raji Abdulrafiu, Sinead Griffin, Ali Hassan , Allison Hatt, Brice Malonda, Kiplangat Sutter
Tutors: George Manyali, Steve Ndengue, Kingsley Obodo, Cecil Ouma, Elvis Shoko
(More advanced students who did more advanced work and also tutored less advanced students.)
Invited speakers: Dr. Moses Rugutt, Deputy CEO, Kenya National Council for Science and Technology, Dr. Happy Sithole, Director, Centre for High Performance Computing (CHPC) South Africa.

Participants: There were 36 participants from nine African countries: Cameroon, Congo, Ethiopia, Ghana, Kenya, Nigeria, South Africa, Tanzania and Zimbabwe. (Many of the students from South African were actually nationals from other African countries.) See photograph below.

Sponsors

* The primary sponsor of ASESMA is the **International Union of Pure and Applied Physics (IUPAP**) through the Commission of Physics for Development (C13) and the Commission of Computational Physics (C20). The Commission on the Structure and Dynamics of Condensed Matter (C10) also supported the School.

* The **International Council for Science (ICSU)** provided a grant for the School.

* A key role was played by the **International Centre for Theoretical Physics (ICTP) in Trieste,** who provided financial and administrative support for the School. Scientists from the ICTP and **Democritos Italian Simulation Center** lectured at the School, and facilitated the use and access of the Quantum Espresso codes, and made these freely available to the participants. There was excellent administrative support for the School by Milena Poropat (ICTP).

* The **International Center for Materials Research (ICMR) in Santa Barbara** provided support for the lecturers and mentors from the USA.

* The **National Institute for Theoretical Physics (NITheP)** paid for the participation of students and lecturers based in South Africa, as well as one lecturer from Europe.

* The **German Academic Exchange Service (DAAD)** provided support for its alumni attending the School.

* The Beijing Computational Science Research Centre (**CSRC)** provided financial support for the School.

* The **National Council for Science and Technology (NCST), Kenya,** provided support for the School. The Deputy Director was in attendance to participate in one of the sessions.

* Chepkoilel University College (Now University of Eldoret) payed for local transport and other finances for the School.

* Further sponsors included the **Division of Computational Physics of the American Physical Society**, the **US Liaison for IUPAP,** and the **Materials Computation Center at the University of Illinois at Urbana-Champaign**.

*** Efforts are underway to obtain support for future Schools. IUPAP has committed to sponsor the series but financial support must be requested for each School. The ICTP has committed support for the 2014 School.**

Summary of the Impacts from CMSG activities

Some of the noticeable impacts to the University of Eldoret and the country at large have been an increased number of the students taking graduate physics in the country as well as more collaborators between Kenyan researchers and industry than before. Indeed government institutions have inquired into the possibility of partnering with universities to train their staff in key areas relevant to them.

The international community has also shown great interest in collaborating with Kenyan scientists in key research projects of mutual interest.

The Kenya government through its relevant arms has recognized the potential of the CMSG in collaborating towards the development of specialized research centres like the nanotechnology centre as well as the establishment of the national physical sciences research institute that is expected to impact on the lives of ordinary Kenyans through research of national strategic relevance.