African School on Electronic Structure Methods and Applications

ASESMA

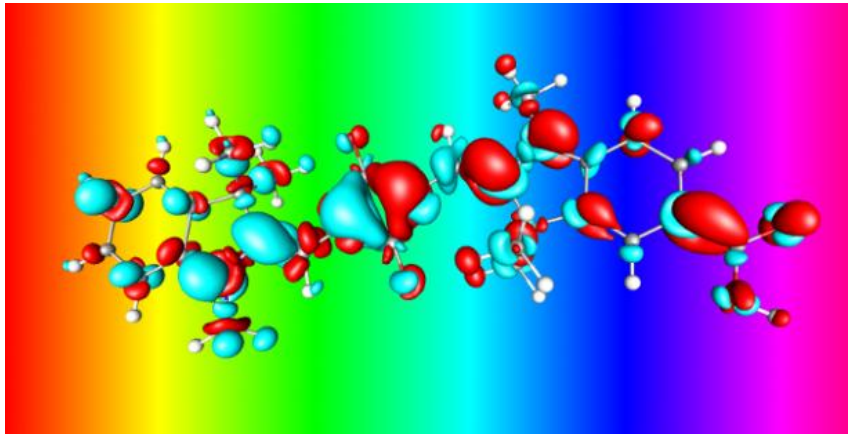
A Biennial Workshop Series - 2010 to 2020

African School series on "Electronic Structure Methods and Applications" – a biennial workshop series from 2010 to 2020

Topics: Electronic structure methods, Molecular dynamics, density functional theory, associated algorithms, general introduction and current challenges in solid state theory and materials science.

Plan:

1. Workshops to be hosted every two years by successive African countries.
2. Each workshop will be focused on a particular theme, e.g. materials for energy, optical properties, defects, surfaces, etc.
3. 4 days with basic lectures + 10 days of hands-on computational work.
4. The hosting institution will provide a networked computer laboratory
5. Different computational packages, freeware is encouraged.



African School series on "Electronic Structure Methods and Applications" – a biennial workshop series from 2010 to 2020

International Advisory Panel

Richard M. Martin – Chair (University of Illinois and Stanford University, USA)
O.O. Adewoye (President, African Materials Research Society)
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Jim Gubernatis (Los Alamos National Laboratory, USA)
Walter Kohn (Kavli Institute for Theoretical Physics, Santa Barbara, USA)
Anthony Leggett (University of Illinois, USA)
Yu Lu (Institute of Physics, Chinese Academy of Sciences, China)
Nicola Marzari (EPFL Lausanne, Switzerland)
Samuel Yeboah Mensah (University of Cape Coast, Ghana)
Bernard M'Passi-Mabiala (Marien NGouabi University, Congo, Brazzaville)
Shobhana Narasimhan (Jawaharlall Nehru Centre for Scientific Research, India)
Chukwuemeka M I Okoye (University of Nigeria, Nsukka, Nigeria)
David Pettifor (Oxford University, UK)
Kennedy Reed (Lawrence Livermore National Laboratory, USA)
Sandro Scandolo (International Centre for Theoretical Physics, Italy)
Wole Soboyejo (AUST, Abuja, Nigeria)
Nicola Spaldin (ETH Zurich)

commentary

Material progress in Africa

Nithaya Chetty, Richard M. Martin and Sandro Scandolo

A school on computational materials science that drew expert teachers and talented participants marks a new approach to the development of research in Africa.

Throughout the African Union, there is tacit understanding of the importance of science in the development of the continent. Although this may be slow to translate into significant improvements, scientific research and education are advancing in a good number of African countries, with improved financial and administrative support. The vast pool of latent talent could be the source of advancement and cooperation, with the potential to overcome political barriers within Africa, strengthen democratic ideals and improve economic and social conditions for all African citizens.

The groundwork is developing for scientific research and collaboration to be on a firmer footing in coming years. An example is the inaugural African School on Electronic Structure Methods and Applications (ASESMA), in which we were involved, held in Cape Town, South Africa, a few months ago. It's a good model for future scientific initiatives, through which African scientists, in partnership with international scientists and organizations, are poised to deliver high-quality science and reap the benefits of increasing investment in science in Africa.

Changing interactions

In the past, the primary mode of scientific engagement between Africa and the rest of the world involved African students and researchers travelling abroad, for education and training or to work in collaboration. The International Centre for Theoretical Physics (ICTP), for example, in Trieste, Italy, has been a 'home away from home' for some twelve thousand African scientists over the past forty years. This means of engagement must continue to grow, of course, especially at laboratories that host highly specialized equipment and facilities.

But today, interaction is shifting towards visits, regional workshops and meetings in Africa itself, with scientists from around the world travelling to Africa to share their knowledge and experience. An important outcome of this is the involvement of more Africans in scientific activity, and an increase in mobility and collaboration within Africa; more African scientists are beginning to talk to each other about scientific problems of mutual interest.

The ASESMA is aimed at bringing young scientists together to foster a stimulating environment, and to develop collaborations and infrastructure for forefront research at the highest level. Why target materials research? It is an area that involves computation — computation that can be done with modest facilities, but with wide-ranging relevance to scientific and technological development, on topics such as materials for solar energy, strong materials and minerals.

Africa has vast reserves of precious minerals. But it needs to move away from simply hauling rocks from deep underground and exporting them to far-flung places. More value stands to be added if the continent invests in establishing its own internationally credible materials research community. African scientists must take a more fundamental approach to understanding material systems, with the view to exploiting their properties for new technical applications that will lead to the development of a materials industry in Africa — bringing with it possibilities for innovation and, ultimately, for development and economic well-being.

Computational studies of real materials are a key part of modern materials research, and such studies are crucial in developing capabilities in Africa. With an improving infrastructure for networking, it is now feasible for African researchers to join in with the international research effort and to contribute to the advancement of science.

NITHAYA CHETTY

Figure 1 | School's out. Participants in this year's African School on Electronic Structure Methods and Applications, outside the African Institute for Mathematical Sciences in Muizenberg, Cape Town.

School days

The ASESMA took place at the African Institute for Mathematical Sciences (AIMS) in Muizenberg, Cape Town, at the end of July — but it was not merely a two-week school. Rather, it is an ongoing programme for networking, education and collaboration in a focused area of research, with the goal of building up a lively, self-sustaining scientific community.

Overseen by a 25-strong international advisory panel (including two Nobel laureates), the school drew more than

ASESMA-2010
17-28 July 2010
AIMS, Cape Town
South Africa

Nature Phys. **6**, 830-832, Nov 2010

2009, page 40). The PhysTEC program is managed by the American Physical Society and the American Association of Physics Teachers and supported by the American Institute of Physics (AIP, which publishes PHYSICS TODAY). At least 17 US physics departments have adopted the program since it began in 1999.

"There's a need for about 1200 new physics teachers per year to meet the demand of the more than 1 million students now taking high-school physics, and we're still only producing 400," says Theodore Hodapp, APS director of education and diversity. Many current high-school physics teachers aren't trained physicists. According to AIP's Statistical Research Center, 54% of the roughly 27 000 high-school physics teachers in the 2008–09 school year did not have a physics degree. That percentage doesn't include those who were subsequently certified to teach high-school physics. "Sometimes it's easy to look at numbers and to overlook what's important, which is making sure that the teacher has the ability to actually teach," says center director Roman Czujko.

"Give us a successful teacher, and we'll teach him or her physics," says Robert Goodman, 2006 New Jersey Teacher of the Year and director of the New Jersey Center for Teaching and Learning, which provides curricula, pedagogical tips, and classroom technologies to local high-school science teachers. The industry CEO turned physics teacher says his approach is to take skilled teachers from any discipline, including from the arts and other humanities, who have an interest in becoming science educators and train them using a curriculum he designed that teaches physics before chemistry and biology. "Physics first" has also been advocated by others, including Physics Nobel laureate Leon Lederman (see his Reference Frame in PHYSICS TODAY, September 2001, page 11). In the year since the New Jersey center started its teacher recruitment and training initiative, Goodman says the number of physics teachers in Newark has already tripled.

The American dream in peril

Programs like Goodman's are preferred by politicians who favor local advancement of education policies. "The federal government shouldn't legislate [education] reform," says Representative Roscoe Bartlett (R-MD), a PhD physiologist and former professor. To promote STEM, the federal government can inspire the nation by inviting scientists to the White House and recognizing them in other visible ways, Bartlett says. "Although most of the Nobel Prize winners in science still come from the US, we aren't producing nearly enough scientists anymore. Now, the bright young kids are going into law and political science. We have enough lawyers and political scientists."

The federal government can partner with local school districts through grants to help teachers prepare for the higher national standards expected for the future, says University of Maryland physicist James Gates, who cochaired the PCAST STEM education report. But no matter who's pulling the education policy strings, "there's a real crisis here," says Gates. "We're not talking about STEM just to produce more scientists and more engineers. We're talking about it in order to give our economy a shot at producing the American dream for future generations. If we don't get this right, the American dream is going to die." **Jermey N. A. Matthews**

Raising the scientific level and networking in Africa

Bringing top scientists to Africa has a greater impact than sending individual African scientists abroad.

"I have never seen so much enthusiasm," says Sinead Griffin, referring to the African School on Electronic Structure Methods and Applications (ASESMA), where she participated as a mentor. "There were hands flying up all the time to get help. No one wanted to leave the computer room in the evenings." Some 40 students and early-career lecturers from eight African countries attended the two-week boot camp last July near Cape Town, South Africa. One of them was Naphtaly Moro of Kenya, who says ASESMA was "an eye-opener to me, for it exposed me to research and experts. The experience is unforgettable to say the least."

The biennial school, which launched last year, and its host, the African Institute for Mathematical Sciences (AIMS), are different approaches with a common goal: Both are part of a small but growing trend to increase the number of educated people in Africa and the level of their education and to create tighter ties among researchers across the continent. Outside of astronomy, ASESMA and AIMS, which offers a program equivalent to the first year of a master's degree, are perhaps the most visible such efforts.

Making science work

Obtaining funding for and maintaining lab equipment are huge challenges in Africa, says ASESMA co-organizer Nithaya Chetty, a physicist at South Africa's University of Pretoria. "So computation is a relatively easy way to make science work here." Electronic structure methods can be applied to many problems relevant to Africa, such as predicting new materials and improving fracture toughness, wear resistance, and other material properties, he adds, and the know-how can be transferred to other disciplines.

"What we are trying to achieve has potential impact on many facets of science and the economy—minerals, materials, computational sciences, energy," says Chetty. After holding a similar school two years earlier, Chetty and others argued that a sustained effort was key to having lasting impact and they arranged to hold ASESMA sessions every two years through 2020. The schools are sponsored by two commissions of the International Union of Pure and Applied Physics and receive financial support from an array of international bodies.

The organizers also introduced a year-round mentoring program. Six mentors—four from the US and two from Africa—attended ASESMA and remain available to the students, interacting mostly via e-mail and Facebook. Griffin, a graduate student in materials science at the University of California, Santa Barbara, says she spends four or five hours a week helping ASESMA students. "Most of the questions are about running [computer programs], but they feed into conceptual questions about the physical systems." About half of the ASESMA 2010 participants continue to work together on a project they started at the school: calculating the transition pressures at which quartz and other materials change structure. What makes ASESMA special, says Chetty, "is mentoring, continuity, and bringing quality scientists to Africa."

RICHARD MARTIN

Participants at last July's African School on Electronic Structure Methods and Applications logged long hours and didn't want to leave the lab in the evenings.

In the past, Chetty says, the primary mode of scientific engagement between Africa and the West was to send African students and scholars abroad. "I don't want to underplay that," he says, "but with Western scientists now traveling to African destinations, the impact is on a larger body of African scientists. It has a greater ripple effect."

Common languages

Neil Turok, AIMS founder and head of the Perimeter Institute for Theoretical Physics in Waterloo, Ontario, says of ASESMA 2010, "It was a great school. The topic was chosen well. They basically showed people in Africa how to use the latest software for calculating band structure in materials. People can take that stuff home with them and use it for their research." But, he adds, "what Africa really needs are solid institutions. Real growth of a strong physics community requires strengthening institutions and creating new ones. Summer schools are no substitute."

The AIMS center in South Africa was founded in 2003 (see PHYSICS TODAY, May 2008, page 25). "We have 50 to 55 students a year from around 20 countries. We feed our graduates to master's and PhD programs across Africa," says Turok. A second AIMS center opened in Nigeria in 2008, and in July 2010 Turok secured Can$20 million ($19.6 million) from the Canadian government to found three new centers—in Senegal, Ghana, and Ethiopia. His goal is to grow to 15 centers. At that point, he says, "we will graduate 750 students a year, and this will completely transform the development of scientific talent in Africa."

Efforts to unify Africa go beyond science, of course. But, says Turok, in overcoming the legacy of colonialism, "math and science are the common languages that overcome religious, cultural, and gender barriers. The biggest single success of AIMS is showing that multicultural diversity is in fact a stimulus and a source of inspiration."

Among other efforts to strengthen intra-Africa scientific cooperation is the formation of the African Physical Society (see PHYSICS TODAY, March 2010, page 25). And if South Africa lands the Square Kilometer Array radio telescope—a final decision between it and Australia is expected in 2012—radio receiving dishes would be installed in Mozambique, Botswana, and other countries. The array, says Chetty, "holds a lot of promise for intra-African collaboration." And science spending is going up. In South Africa, for example, it is now 0.8% of the gross national product, up from 0.65% a few years ago. Still, he says, "there is not an awful lot occurring on a continental scale. And it's often ad hoc in nature. I hope that establishing a few success stories with outside help will generate momentum for further developments in science in Africa." **Toni Feder**


Algiers
Tunis
Casablanca
Rabat
Oran
Constantine
TUNISIA
Mediterranean Sea
MOROCCO
Marrakech
Bechar
Tripoli
Banghazi
Alexandria
Cairo
Western Sahara
El Aaiun
ALGERIA
LIBYA
EGYPT
Al Jawt
Aswan
Tamanrasset
MAURITANIA
MALI
NIGER
Faya-Largeau
Port Sudan
Nouakchott
Nema
Lombouctou
Agadez
CHAD
ERITREA
Asmara
Dakar
SENEGAL
Khartoum
Niamey
Zinder
Al Fashir
DJIBOUTI
Djibouti
THE GAMBIA
Bamako
BURKINA
N' Djamena
Berbera
GUINEA BISSAU
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Ouagadougou
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Maiduguri
SUDAN
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Beira
Windhoek
BOTSWANA
Toliara
Gaborone
Pretoria
Maputo
Luderitz
Johannesburg
Mbabane
SWAZILAND
Maseru
Durban
LESOTHO
SOUTH AFRICA
Cape Town
Port Elizabeth

AFRICAN SCHOOL ON ELECTRONIC STRUCTURE METHODS AND APPLICATIONS (ASESMA-2012)

Location: Chepkoilel University College, Eldoret, Kenya

Dates: May 28 - June 8, 2012

Directors:
George Amolo and Nicholas Makau (Chepkoilel)
Richard Martin (U. Illinois, USA)
Nithaya Chetty (U. Pretoria, South Africa)
Sandro Scandolo (ICTP)

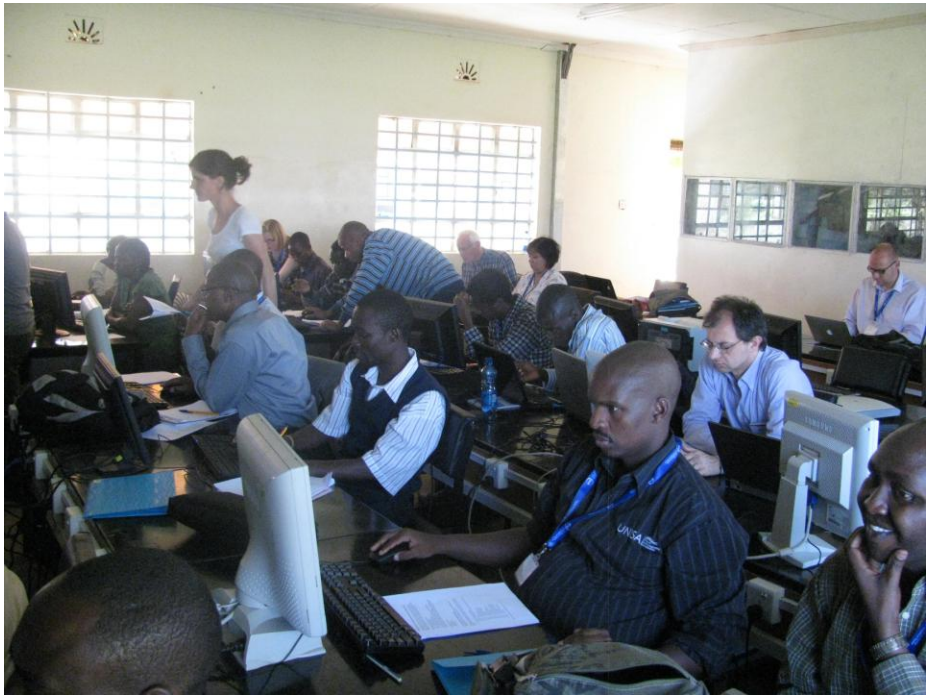
Special focus:
Materials for energy applications

Photovoltaics
Catalysis
Hydrogen storage
…

ASESMA 2012

Moi University
Eldoret,Kenya

May 29, 2012



ASESMA 2012 -- The Students

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 Africa were actually nationals from other African countries

ASESMA 2012 -- The Lecturers

Lecturers:
Thomas Bligaard (Stanford)
Roberto Car (Princeton)
Mark Casida (Grenoble)
Ralph Gebauer (ICTP)
Stefano de Gironcoli (SISSA)
Paolo Giannozzi (Udine)
Daniel Joubert (Wits)
Lev Kantorovitch (King's College)
Ryo Maezono (Tokyo)
Bernard M'Passi-Mabiala (Brazzaville)
Shobhana Narasimhan (Bangalore)
Annabella Selloni (Princeton)
Renata Wentzcovich (Minnesota)

Special guests / 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.

Mentors - A critical link between lecturers and students

Assisted students on a one to one basis, allowing each to progress at his own rate

ASESMA 2012

The Mentors

Ali Hassanali
ETH Zürich
(Switzerland)

Alison Hatt
LBNL
(USA)

Brice Malonda
Brazzaville
(Congo)

Cecil Ouma
U of Pretoria
(South Africa)

George Manyali
U of Wits
(South Africa)

Abdulrafiu Raji
ICTP
(Italy)

Steve Ndengue
U of Douala
(Rep. Cameroon)

Kingsley Obodo
U of Pretoria
(South Africa)

Sinéad Griffin
ETH Zurich
(Switzerland)

ASESMA 2012

Highlights

A number of projects were proposed after the 1st week of lectures, and the participants were grouped according to their project interests. The mentors assisted the participants with their projects. Each group made a presentation of their project work at the end of the School.

During the first week, an exciting 2-hour public lecture on Geophysics was given by Renata Wentzcovich (Univ Minnesota). The attendees included university staff and students, together with students from schools neighboring Chepkoilel University College.

ASESMA 2012 - Sponsors

*** IUPAP C-13 and C-20: 7,000 Euro**
*** IUPAP C-10: 6,000 Euro**
*** ICTP: 20,000 Euro**
*** Democritos / CNR: Travel expenses for three lecturers**
*** The International Center for Materials Research (ICMR), Santa Barbara: 40,000 USD for US speakers/mentors**
*** The National Institute for Theoretical Physics (NITheP) paid for the participation of students based in South Africa.**
*** Division of Computational Physics of the American Physical Society: 4,000 USD**
*** US Liaison for IUPAP: 6,000 USD**
*** Materials Computation Centre at the University of Illinois at Urbana-Champaign: travel expenses for one lecturer**
*** The German Academic Exchange Service (DAAD) provided support for its alumni attending the School.**
*** The Chinese Supercomputing Research Centre (CSRC): 10,000 USD**
*** The National Council for Science and Technology (NCST), Kenya, provided local support**

ASESMA 2012
Financial Support

SIGNIFICANT GRANT RECEIVED IN APRIL 2012

From

INTERNATIONAL COUNCIL FOR SCIENCE (ICSU)

10K Euros of ICSU Grant used to support the school in Kenya

20K Euros of the ICSU Grant to be used to help support follow-up actions

Mini-Workshops

ICSU
International Council for Science

ICSU
International Council for Science

Mini Workshop

Khartoum University
Khartoum, Sudan
January 19–28, 2013

Students from Sudan, South Sudan and Kenya

Mini-Workshop at Khartoum University

Introduction to Basic Theory with emphasis on Practical Calculations.

Topics:

- Introduction to inter-atomic potential methods
- Point defects in solids using GULP
- Introduction to molecular dynamics
- Applications of GULP
- Introduction to Density Functional Theory
- Electronic structure calculations with Quantum ESPRESSO code
- Simulations of metallic system
- Simulations of magnetic system
- Structural optimization
- Surfaces

The workshop in Sudan included students from South Sudan who now will begin collaborating with Sudanese scientists. Noteworthy considering the recent history of that region.

Mini Workshop

Braazaville,Congo

April, 2013

ASESMA is on Facebook!

There is also a Monthly Newsletter

ASESMA
A Biennial Workshop Series From 2010 to 2020

Potential Hosts for Future Schools

Plans for ASESMA 2014 to be held in Brazzaville, Congo - a Francophone country

The African University of Science and Technology (AUST) in Abuja, Nigeria will host in 2016

Goal: Build a Critical Mass of Expertise and Capabilities in Computational Materials Science in Africa