

Schooling Africa: Computational Materials Science education and research

N. Chetty

Physics Department, University of Pretoria, Pretoria, 0001, South Africa and National Institute for Theoretical Physics, Johannesburg, 2000, South Africa

Richard M. Martin

Stanford University, Palo Alto, California, USA and University of Illinois at Urbana-Champaign, Urbana, Illinois, USA

Nithaya.Chetty@up.ac.za

Abstract. The African School of Electronic Structure Methods and Applications (ASESMA)^[1-7] is a series of workshops held every two years in different sub-Saharan countries, designed to foster a collaborative network for research and higher education in Africa. Participants are drawn from across the continent through a competitive process, and the lecturers and mentors are outstanding scientists from across the world including Africa. ASESMA is administered by the International Centre for Theoretical Physics (ICTP), and the primary sponsor is the International Union of Pure and Applied Physics (IUPAP). The core guiding principle is that computation makes it possible for world-class research to be done with modest investment, and it is an essential part of education for the future. The skills acquired are useful for teaching at the university level and are transferable to other disciplines. The participants are the teachers who will educate future generations of African scientists.

1. Introduction

Africa is richly endowed with critically important mineral deposits, which can be the basis for growing its scientific research capacity with important benefits for people development and for the economy. Developing materials science as an educational and research endeavour in all its different facets in Africa should be a priority. And indeed it is in many parts of the continent given the many different materials science initiatives that are on-going in Africa, but there is still a long way to go before Africa can take its rightful place as a leader in this important area.

The recent meeting of the African Materials Research Society Meeting held in Gaborone, Botswana in December 2017 was very successful, and gave a strong indication of the growing field of materials science in Africa^[1] (The present paper is largely taken from the article on ASESMA that was delivered at this meeting.). An important observation was that this is being done in partnership with many international scientists and institutions, and this augurs well for the future. Examples of the partnerships, include the outstanding long term support of the International Centre for Theoretical Physics (ICTP)^[8], the International Union for Pure and Applied Physics (IUPAP), for example through its support of the LAMMP^[9] network, and the Royal Society in the UK, and more recent developments such as the Pan

African Materials Institute (PAMI), the Joint United States African Materials Institute (JAUMI), SciBridge, led by North Carolina State University, and the African Materials Science and Engineering Network (AMSEN). A new development is the establishment of the East African Institute for Fundamental Research (EAI FR) in Kigali, Rwanda, which is affiliated to the ICTP. EAI FR has prioritised condensed matter physics, geophysics, high performance computing amongst other areas of physics, which will provide a centre for activities across Africa as well as strong research in the institute. There needs to be more coordination between these different initiatives to ensure that ‘the whole is greater than the sum of the individual parts’.

The African School for Electronic Structure Methods and Applications (ASESMA)[1-7] is one such successful initiative that has been in existence for the past decade. ASESMA has shown that it is possible to build a network across sub-Saharan Africa with world-class research with a relatively low budget. The greatest asset is the commitment of the lecturers and mentors, the team-work of the local organizers and the idealism of the participants who rank amongst the brightest of young minds from Africa, many of whom come from impoverished backgrounds but still dare to reach for the stars.

2. The importance of computational materials science in Africa

Materials Science is primarily an experimental endeavour and an empirical science. However, modern experimental equipment is costly, and the service and maintenance of sophisticated equipment requires specialised skills and substantial financial resources. Computing, on the other hand, is relatively cheap and world-class research can be done without great cost or local facilities. Computer networking is becoming more reliable in Africa. The internet in Africa is operating reasonably reliably with speeds of up to 10Mbits/sec in most places. Optical fibre and faster bandwidth is available in a select number of cities on the continent.

Computational Materials science is now an integral part of research that greatly expands the possibilities for creating new materials, optimizing performance in technological applications, and understanding the basic properties at a fundamental level. Freeware production codes in materials science modelling are becoming more readily available, with better online support. Increasingly, experimentalists are using computing methods to analyse their results, which substantially increases the need – and the opportunities - for computational materials science in Africa.

Computation is not only a useful tool that is an integral part of every area of science and technology, it also is the intellectual frontier that brings together the sciences, engineering and technology. There is great cross fertilization between basic research and technological applications in chemistry, physics and biology that are brought together in computational materials science. For example, the same codes can treat solids – minerals, semiconductors for solar energy, components of batteries for energy storage, etc. – and molecular systems for light harvesting and drugs for diseases that have traditionally been the provenance of chemistry and biology. These are integral parts of computational methods to study complex reactions and entire systems.

Although ASESMA has been mostly focused on teaching electronic structure methods for applications in materials science, there is a move to expand its scope to the area of biological sciences. In particular, many of the methods used in solid-state physics have been successfully used in the area of soft-condensed matter and computational biology.

Computational materials science is an important way to begin to build materials science capacity at African institutions particularly where resources are limited. Great science can be done with small computers, but some problems require large computers. The Centre for High Performance Computing (CHPC) in Cape Town has been making computing resources available for African scientists, but it is

becoming over-subscribed. It will be very beneficial if African scientists can have greater access to international supercomputing facilities from around the world

3. The African School of Electronic Structure Methods and Applications (ASESMA)

The African School of Electronic Structure Methods and Applications (ASESMA) is a series of workshops held every two years in different sub-Saharan countries, designed to foster a collaborative network for research and higher education in Africa. Participants are drawn from across the continent through a competitive process, and the lecturers and mentors are outstanding scientists from across the world including Africa. The administration of ASESMA is managed by the ICTP.

ASESMA is sponsored for the years 2010 to 2020 by the International Union of Pure and Applied Physics (IUPAP) as a joint mission of the Commissions on Physics Development (C13), Computational Physics (C20), Physics Education (C14) and the Structure and Dynamics of Condensed Matter C(12), and it is supported by the International Centre for Theoretical Physics, the National Research Foundation in South Africa, the U.S. Liaison Committee for IUPAP, the American Physical Society, the US National Science Foundation, and as well as a number of international organizations and industries.

The core guiding principle is that computation makes it possible for world-class research to be done with modest investment, and it is an essential part of education for the future. The skills acquired are useful for teaching at the university level and are transferable to other disciplines. The participants are the teachers who will educate future generations of Africans.

The focus of ASESMA is computational methods and applications of electronic structure, chosen because it is an important field that is narrow enough to build up a network for joint work and collaboration, yet broad enough to span the range from fundamental physics to applications in materials science, chemistry, biology and many other fields. In each workshop participants learn the basic theory and computational methods with hands-on computing, and each participant is involved in a project in an area of current research that can be continued after the school. The main applications are to materials that are crucial for many areas of technology, including solar energy and the vast reserves of minerals and materials mined in Africa. The Quantum Espresso (QE) codes are primarily used because these are freely available and are versatile with excellent online documentation. The developers of QE are strongly committed and actively involved in ASESMA.

A novel aspect of ASESMA is the involvement of mentors who are often young experienced people at the advanced stages of their doctoral degrees or postdoctoral fellows, often very keen and excited to be a part of a team that is making a difference in Africa. Initially there was much reliance on recruiting mentors from abroad, but increasingly now there is developing sufficient expertise in Africa that more mentors are being drawn from the continent itself. This is an important sign of progress.

The schools are not only concerned with technical issues; an important part of the mission is devoted to life skills in the research environment: finding a good problem, writing a paper; writing a proposal for funding; identifying good collaborations; being a good teacher and mentor for younger people. In addition, there are serious discussions of issues like how to deal with sexual harassment and discrimination in the workplace. There often are general, overview talks held after dinner to enthuse participants and to give them an idea of the broader picture of materials science in the world.

A hallmark of ASESMA is the camaraderie and joyful interactions among participants, mentors, and lecturers. It is traditional to have a special dinner on the last night at the School where prizes are awarded in categories, including the most improved, most helpful, most joyous, etc. all-round performance, etc. There is a palpable feeling of fulfilment amongst the mentors and lecturers of knowing that they are

making invaluable contributions to a part of the world that is in need, and of working with bright young African students and young faculty who represent the future.

The important need now is for funding for research, for ASESMA participants to attend international meetings, and for short visits to international institutions that are all essential for scientists to participate fully in the global community.

4. Discussion

With the different materials science initiatives that are underway, including the African School of Electronic Structure Methods and Applications (ASESMA) reported above, there is need for more coordination, more information sharing and cooperation between the different activities so that the full impact on the African continent can be greater than the sum of the individual efforts. More reporting of positive stories^[10] and highlighting of role models, especially of successful women is needed.

There is a need for more grassroots, bottoms-upwards and one-on-one initiatives with attention to excellence in training and research, focussed on working on current exciting and relevant publishable problems. The training of students should be done in a *milieu* of excellence while aspiring to the highest international standards of scholarship. It is not in anyone's interests to compromise on quality. African physics departments should be strongly coupled to the outside world, and the idea of twinning is a demonstrable way to build much needed capacity. There is a need for more mentorship and coaching to be a successful researcher, for example scientific integrity and the responsible conduct of research training in science education is important in this context.

The establishment of physical societies within a growing number of African countries is an achievable goal and should be vigorously pursued. The African Physical Society (AfPS) is being renewed with a continental-wide brief that should play more of a coordinating role, and could be the voice of physics in Africa.

The development of materials science in Africa is taking place in a constrained financial environment. Salaries are generally poor, and funding for research grants and studentships are limited. This needs to improve, and African governments need to contribute more funds for education and research. There needs to be strong and sustained advocacy for support for materials science in Africa. This will come from a more concerted effort at public understanding of materials science, and engagements with policy makers at the highest levels. Key statistics need to be gathered that can be used for marketing the importance of materials science development to decision makers and the broad public.

In this regard, the Physics in Africa project^[11] that was a joint effort by members of the American Physical Society, the European Physical Society, the Institute of Physics, the South African Institute of Physics, the International Centre for Theoretical Physics, and the Materials Research Society gives much-needed evidence-based direction for taking physics development in Africa to the next level. The key outcomes of this project were centred on: (i) Communication, (ii) Physical societies, (iii) Experimental physics, (iv) Physics education, and (v) Physics and society. These topics have been adequately addressed in the project report. This initiative will benefit materials science in Africa.

Despite the difficult financial environment for materials science in Africa, there are nevertheless opportunities that need to be better exploited for financial resources, for example from the Newton Fund, the European Union, the US National Science Foundation, the National Research Foundation of South Africa, etc. There often isn't a single source of funds for a major materials science initiative, and much work needs to be done to secure money from multiple sources from different organisations around the world to make things happen. This requires dedication and persistence. Reporting this information in

the various news outlets mentioned above of international organisations sympathetic to materials science development in Africa will greatly assist initiators of new projects in Africa.

Inter-institutional partnerships and agreements between African and Western organisations will be an important step-up from one-on-one partnerships mentioned above, and should be a goal for taking materials science cooperation to a higher level with the potential for more sustained impact. This will happen naturally when materials science research groups at African institutions begin to be established with greater success, and this will take time.

Historically, culturally and politically, there have been divisions between English-speaking and French-speaking Africa. It is important for scientists to look beyond this divide so that science development can be seen to be a truly pan-African endeavour with benefits to all. Materials science has the potential for leading in this way.

African scientists are more likely to travel to a Western destination than to another African destination to collaborate; incentives should be created for more intra-African mobility and collaborations in materials science, even if only on a regional basis. Travel permits should be issued with greater freedom for visiting scientists.

There is a need for more regional meetings, conferences, workshops and schools in materials science in Africa. This will help address the issue of isolation faced by many African scientists. Western scientists visiting African institutions influence a larger number of African scientists, students and the African public than travel in the opposite direction. This also gives traveling Western scientists first-hand experience in understanding the often difficult circumstances that many African scientists work under.

This is not to diminish the importance of African scientists traveling to Western institutions as this must continue unabated since this is the most effective and time-honoured means of developing talented African individuals. However, it should be noted that the current political environment in many places in the West is becoming increasingly difficult for visitors from the developing world and this burgeoning problem needs to be better recognised. Furthermore, the economic environment is also creating a hurdle for many scientists from the developing world to journey to the West.

There can now be much better use of web-based teaching with video courses but these need to be geared for different levels of students, and perhaps with example applications more relevant to Africa. Social media can be better used to communicate and to network.

5. Concluding remarks

ASESMA has shown that it is possible to build a network in a particular scientific area across sub-Saharan Africa with world-class research with a relatively low budget. It already is expanding to involve more chemistry and materials science, with an introduction into biological systems. These are steps toward fulfilling the vision of building African Networks for Computational Materials and Biological Sciences. The greatest asset is the commitment of the lecturers and mentors, the team work of the local organizers and the idealism of the participants who rank amongst the brightest of young minds from Africa, many of whom come from impoverished backgrounds but still dare to reach for the stars. This is an inspiring story for all who get involved.

The core guiding principle is that computation makes it possible for world-class research to be done with modest investment, and it is an essential part of education for the future. There is tremendous

goodwill of scientists world-wide and there is great potential in the young people of Africa who only need the opportunities to take part in the global community of science!

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- [11] See <http://www.saip.org.za/index.php/physics-in-africa-survey>