

GRANTS PROGRAMME 2012

APPLICATION FORM

(Valid for ICSU Members only)

(Applications must be submitted electronically to rohini@icsu.org)

Deadline for submission is 1 December 2011

Lead applicants*¹ may submit no more than one application. **A ceiling of Euro 30,000 is imposed on all applications.**

Project title: African School of Electronic Structure Methods and Applications (ASESMA)

**Requested amount (€):30 000
(Maximum Euro 30,000)**

Applicants:

Lead Applicant:

Organization: IUPAP

Contact name & Designation: Prof Robert Kirby-Harris, Secretary General

Email address: secgen.iupap@iop.org

Supporting Applicants:

Organization: ICSU Regional Office of Africa [*ICSU Regional Office*]

Contact name & Designation: Dr. Edith Madela-Mntla, Director

Email address: director@icsu-africa.org

Organization: Consiglio Nazionale delle Ricerche (CNR, Italy) [*ICSU National Member*]

Contact name & Designation: Prof. Stefano de Gironcoli, Director, IOM-Democritos Center

Email address: stefano.degironcoli@democritos.it

Organization: Academy of Sciences for the Developing World (TWAS) [*ICSU Scientific Associate*]

Contact name & Designation: Prof. Romain Murenzi, Executive Director

Email address: EDoffice@twas.org

Other partners:

The Abdus Salam International Centre for Theoretical Physics (ICTP) / UNESCO

¹ (ICSU Scientific Unions, Interdisciplinary bodies)

International School for Advanced Studies (SISSA), Italy
International Centre for Materials Research (ICMR), USA
US IUPAP Liaison Committee
Division of Computational Physics of the American Physical Society
University of Illinois Materials Computation Center
Beijing Computational Science Research Center
South African National Institute of Theoretical Physics (NITheP)
South African National Research Foundation (NRF)
South African Department of Science and Technology (DST)
South African Institute of Physics
South African IUPAP Liaison Committee
Centre for High Performance Computing (CHPC), South Africa
Centre of Excellence in Strong Materials (CoESM), South Africa
Moi University, Kenya

How will this proposal address ICSU's strategic priorities as defined for the grants programme:

- *Capacity Building and Science Education:* ASESMA is novel in the manner in which continuity is built into the School series. There is on-going interaction by mentors and lecturers with the School participants for significant periods of time after the School. Over the next ten years, the School will move through various African countries on a biennial basis. This will ensure that this research endeavour will take firmer root within Africa, that networks will be built and that critical mass will be created where none or very little currently exists.
- *Science and Technology for Sustainable Development:* ASESMA will focus on computational quantum mechanics methods applied to materials for sustainable energy applications, including photovoltaics, artificial photosynthesis, fuel cells, and batteries. This has the potential of adding economic value to the vast reserves mined in Africa.
- *Dissemination of data/Information:* hands-on computational exercises will be carried out within a Linux computational laboratory running state-of-the-art open source software.
- *Emerging Science-Creation of New Knowledge:* ASESMA will cover computational advances at the boundary between physics, chemistry, and materials science

Project plan

- Objectives

The African School Series on Electronic Structure Methods and Applications aims to strengthen the field of computational material science in Africa by focussing on the fundamentals of the theory, algorithms and computation for properties of materials of great interest in Africa. The School involves doctoral students and young researchers, includes educational opportunities, and provides international-quality mentorships for research projects on a range of research problems in computational material science. This endeavour has the potential to add economic value to minerals and materials relevant to Africa. The School has a strong pedagogical component, which develops the field of computational material science, and impacts on other cognate disciplines such as mathematics, physics, chemistry, material science, and computation, and in areas of the mainstream economy, with significant impact on the African continent. This ICSU grant is especially targetted at

strengthening networking, collaborations and mobility involving African scientists during the 2012 School and for the first months of the period between the 2012 and 2014 Schools. The involvement of international mentors and senior scientists in this exchange aspect of the programme is critical. We have identified that providing support between Schools is exactly what is required to ensure the long-term sustainability of the programme. This is precisely what is lacking from the vast number of other scientific programmes in Africa. It is anticipated that there will be increased quality in graduate student supervision, and significant impact on quality research outputs as measured by publications in international journals and presentations at international conferences by African scientists.

- Project description

ASESMA Scientific themes

Developments of new theoretical methods, algorithms and widely available codes have brought a new era in computational materials science. This is a field of active research today because it is making possible new understanding and abilities to predict properties of materials. Because of the advent of faster, cheaper computers, new algorithms, and the availability of open source software, such as the Quantum Espresso Codes, there is a world-wide community of scientists developing new methods and carrying out research on important materials problems. With improving networking infrastructure, it has now become viable for African researchers to join in on this exciting international research effort.

The methods stressed in initial Schools will involve density functional theory, which makes possible calculation of materials properties from the fundamental laws with no parameters, and the methods pioneered by Car and Parrinello, which make it feasible to move atoms to determine structures and bonding of molecules and solids. It is now possible to make quantitative calculations for complex systems such as surfaces and interfaces critical for solar energy applications, carbon nanotubes with defects, minerals, transition metal alloys with strong metal-carbon, metal-nitrogen, etc, bonds that are crucial for the strength of materials. Electronic, magnetic and optical properties of materials as well as stability and strength can now be computed, all with the same theoretical methods and the same computational codes. Quantitative calculations make it possible to work hand-in-hand with experimental studies and technological developments. This opens a vast terrain for extensive studies for materials for their scientific and technological value.

The theme of the 2012 School will be materials for sustainable energy production and storage. This is a very broad area that is particularly appropriate for Africa. Specific types of problems include transparent conductors for solar cells, surfaces and interfaces of materials for electrochemical applications, photovoltaic properties of organic films on oxides, photocatalyzed hydrogen production, hydrogen storage, and more generally structures of minerals.

Programme of ASESMA 2012

The 2012 School will be held at Moi University, in Eldoret, Kenya. The first few days will involve basic lectures, including tutorial work, on topics in physics and computational physics that are relevant to the School theme. International experts will be invited to lead discussions on current challenges in solid state physics and material science. Thereafter, for the following days, the School will be focused on hands-on computational work. For these purposes, the hosting institution will provide a networked computer laboratory comprising about 40 computers running Linux with technical support. The School will cater for approximately 40 students, drawn from young faculty and doctoral students from across Africa.

Beyond ASESMA 2012

Strengthening networking, collaborations and mobility involving African scientists during the period of time between the 2012 and 2014 Schools is one of the main targets of this proposal. This will be achieved by taking a series of concrete actions starting immediately after the end of the 2012 School. Experience with the 2010 School has shown that the first six months after the event are crucial for the initiation of collaborative actions. We will set up a team of mentors and lecturers available to travel to meet with small groups of participants in Africa to assist and lend support for their on-going work. A selection of participants in the 2012 and 2010 Schools will be invited to visit mentors, lecturers and/or other international institutions to continue with collaborations. Participants will also be encouraged to attend international conferences, and in particular international workshop on electronic structure methods and applications to present their work (several such workshops are held annually or biannually in Europe, North America, Latin America and Asia). Small workshops on a regional basis in Africa for follow-up studies will also be organized jointly with local institutions.

ASESMA Management

The School series is managed by an International Advisory Panel chaired by Prof Richard Martin (Univ. Illinois) and whose members are listed below:

International Advisory Panel

1. Richard M. Martin, Chair (University of Illinois, USA)
2. O.O. Adewoye (African Materials Research Society)
3. Mebarek Alouani (IPCMS, Strasbourg, France)
4. George Amolo (Moi University, Kenya)
5. Stefano Baroni (SISSA and Democritos, Trieste, Italy)
6. Peter Borchers (Birmingham, UK)
7. Roberto Car (Princeton University, USA)
8. Richard Catlow (Royal Society, UK)
9. XinGao Gong (Fudan University, China)
10. Jim Gubernatis (Los Alamos National Laboratory, USA)
11. Walter Kohn (Kavli Institute, Santa Barbara, USA)
12. Tony Leggett (University of Illinois, USA)
13. Yu Lu (The Institute of Physics, Chinese Academy of Sciences, China)
14. Nicola Marzari (EPF Lausanne, Switzerland)
15. Samuel Yeboah Mensah (University of Cape Coast, Ghana)
16. Bernard M'Passi Mabiala (Marien NGouabi University, Congo, Brazzaville)
17. Shobhana Narasimhan (Jawaharlal Nehru Centre for Scientific Research, India)
18. David Pettifor (Oxford University, UK)
19. Kennedy Reed (Lawrence Livermore National Laboratory, USA)
20. Sandro Scandolo (International Centre for Theoretical Physics, Italy)
21. Wole Soboyejo (Princeton University, USA and African Materials Research Society)
22. Nicola Spaldin (ETH, Zurich, Switzerland)
23. Ahmadou Wague (Universite Cheikh Anta Diop, Senegal)

The 2012 School is managed by a Local Organising Committee chaired by Dr George Amolo and whose members are listed below:

Local Organising Committee

1. Dr. G. O Amolo (Chair LOC) - Moi University
2. Dr. N. Makau (Secretary LOC) – Moi University
3. Dr. N. M. Wambua - Moi University
4. Prof. S. Rotich – Moi University
5. Prof. B. Wishitemi - Moi University – DVC -Research & Extension.
6. Dr. C. Maghanga - Kabarak University
7. Prof. J. Mwabora - Nairobi University
8. Prof. Gateru - Methodist University – Kenya.
9. Prof. J. Okumu - Kenyatta University
10. Mr. D. Ngigi - National Council For Science and Technology (Kenya)
11. Dr. Z. Mapelu - Moi University.
12. Cleophas Wawire - Catholic University of Eastern Africa

- Relevance to review criteria

Innovative nature - The School is novel in the manner in which it builds continuity, and in a location that moves through the African continent over the next ten years. There is a strong pre-School and post-School aspect that helps to entrench the research endeavour and strengthen research productivity. Here, the mentors play a significant role, and this ICSU grant application is especially targeted at achieving the networking and collaborations for the two year period between the 2012 and 2014 ASESMA Schools. Mentors travel to African destinations to lend support to burgeoning research groups. Individual African scientists travel to foreign destinations to interact with mentors and lecturers of the School to gain assistance in their research work. African scientists travel to other African destinations to interact with African scientists and to work on research problems of relevance to Africa. Small workshops are held in Africa on a regional basis to assist with the continuity of the research focus areas.

Interdisciplinary and international nature – The methods are applicable to physical, chemical, materials and biological systems, and thus bring together researchers from a wide range of disciplines. The computational skills acquired are transferable to other disciplines and to the mainstream economy. The lecturers are drawn from Africa and other international institutions.

Visible and measurable outputs - In post-School workshops, participants work specifically on research projects that culminate in international quality publications. The internet is used to facilitate collaborations and networking, and a visible output is increased intra-African mobility, cooperation and collaborations, as well as quality graduate student development.

Relevance to the ICSU strategic plan 2006 to 2011 – The School series is strongly aligned with building a strong scientific foundation in a changing world, building for the future of African science and utilizing and strengthening the current structures. Priorities of the ICSU regional office – The ICSU-Africa Office has endorsed this project (see letter of endorsement).

Young scientists, women scientists, scientists from the developing world - The School involves graduate students and young faculty and researchers drawn from across Africa. A special effort is made to attract African women participation.

- Targeting of priority groups

The School Series targets doctoral students and young faculty and researchers drawn from the African continent, and there is a concerted effort to attract African women participation. A cohort of active participants are networked and linked up with international mentors, especially during the period inbetween Schools to ensure continuity and productivity. International mentors will visit small research groups in African countries and will host small workshops focused on specific research problems during the period of time between Schools. This will ensure that small groups of researchers working in isolation have a real opportunity to flourish with their work.

Work plan

The 2012 School will take place from in May/June at Moi University, Eldoret, Kenya. This funding proposal to the ICSU grants programme is for the 2012 School and for the first six months after the School.

| January - April 2012 | |
|--|---|
| ASESMA Work plan | ICSU support |
| ASESMA 2012 School preparation, including selection of lecturers, web site, online application procedure, selection of participants, invitation letters and travel assistance. | Travel expenses of 5 selected participants from African countries outside Kenya |

| May-June 2012 | |
|--|---|
| ASESMA Work plan | ICSU support |
| ASESMA 2012 held in Kenya on May 28 - June 8. First week: lectures of a general and pedagogical nature focussed on basic solid state theory. Prof Richard Martin will lead these discussions which will involve other local and international lecturers. One or two public lectures will be given for the benefit a wider audience. Second week: hands-on computational exercises within a Linux computational laboratory running open source software such as Quantum Espresso. The students and lectures will be living in close quarters which will ensure that there is ample time allocated for late night discussions and tutorial group exercises. | Living expenses of 5 selected participants from African countries outside Kenya |

| June-December 2012 | |
|--|--|
| ASESMA Work plan | ICSU support |
| Mentors and lecturers to travel to meet with small groups of participants in Africa to assist and lend support for their on-going work A selection of participants to visit mentors, lecturers and/or other international institutions to continue with collaborations. A selection of participants to attend an international | Ten travel grants of about 1000 Euro to African students to visit international collaborators and attend international conferences/workshops. Ten travel grants of about 500 Euro to African students and |

| | |
|--|--|
| <p>conference(s) to present their work. A selection of participants to attend an international workshop on electronic structure methods and applications. Small workshops on a regional basis in Africa for follow-up studies.</p> | <p>young scientists to attend regional workshops. Five travel grants of about 1000 Euro to international lecturers and mentors to visit small groups of African scientists. Local support for regional workshops</p> |
|--|--|

Expected results

The ICSU grant will enhance the stature of the African School Series on Electronic Structure Methods and Applications, and will help ensure that for the next ten years the School organisers will be able to leverage funds from various other sources, especially including local sources. This will go a long way toward securing the School for the next decade, which is what is planned.

We expect strong networking and collaborations to develop within Africa itself, and for there to be increased intra-African mobility as a result. This ICSU grant is especially targetted at strengthening networking, collaborations and mobility involving African scientists for the long periods of time between ASESMA schools. The involvement of international mentors in this aspect of the programme is critical. We have identified that providing support between Schools is exactly what is required to ensure the long-term sustainability of the programme. This is precisely what is lacking from the vast number of other scientific programmes in Africa. The field of computational material science will grow in substance within Africa, which will help strengthen the foundational disciplines such as mathematics, physics, chemistry, materials science and scientific computing. Students will have access to freeware software within an opensource environment. These attributes make computing very accessible for scientists in the developing world, especially with the advent of improved bandwidth for internet connectivity, and so an important outcome is the strengthening of computing and computing resources in general on the African continent.

There is an expectation that graduate student development will grow in numbers and in quality, and that there will be an increase in quality publications by African scientists in international journals and an increase in presentations at international conferences by African scientists.

The potential exists for there to be meaningful contributions to the fundamental understanding of materials of relevance to Africa, with a resulting impact on the benificiation of the vast reserves of minerals and materials mined in Africa. This will contibute significantly to the development of world-class materials science on the African continent, with unlimited economic value for the continent.

The Role of Supporting Applicants and Other collaborative partners

- IUPAP (Lead Applicant)

The IUPAP Commission on Physics for Development (C13) is the primary sponsor of ASESMA 2012, in collaboration with the IUPAP Commission on Computational Physics (C20), and with the endorsements by the IUPAP Commissions on Physics Education (C14) and Structure and Dynamics of Condensed Matter (C10). The IUPAP General Assembly has endorsed the School Series and has committed 7000 Euros for the 2012 School.

- ICSU Regional Office in Africa (Supporting Applicant)

ICSU ROA - plays a role of providing guidance in identifying experts and scientists from the region who will be involved in the implementation of this project. The Office will facilitate and foster links between IUPAP and the already existing African national research and educational networks as well as providing guidelines for action agendas and rendering administrative support in organising the implementation of the project. Will promote the activities of the ICSU family in Africa. Will avail staff for any service that may be required, within the limits of its capabilities, for the implementation of the project.

- Academy of Sciences for the Developing World (TWAS) (Supporting Applicant)

TWAS expressed interest in supporting the school in the framework of an agreement with ICTP. However the request reached ICTP too late for the inclusion of the school in the list of activities co-sponsored by TWAS.

- Italian National Research Council (CNR) (Supporting Applicant)

CNR's DEMOCRITOS National Simulation Center, Trieste, Italy coordinates the computational laboratories, makes available the Quantum Espresso code, offers technical expertise in the use of the codes and generally lends support in density functional methods. Democritos provides funds for the support of the travel expenses of their own lecturers and tutors .

- The International Centre for Theoretical Physics (ICTP) (Partner)

ICTP funds and coordinates African (non-Kenyan) participation in ASESMA2012. Sponsors lecturers. Maintains the School website. Provides leadership and oversight for the School. Provides secretarial support in the preparatory stages.

- International Center for Materials Research, Santa Barbara, USA (Partner)

ICMR provides funding for lecturers and mentors for the School. Provides postdoctoral fellows to act as mentors for the School. Assists with networking and communication with School participants, especially after the School, e.g. the ASESMA electronic newsletter.

- National Institute for Theoretical Physics, South Africa (Partner)

Funds and coordinates South African participation in ASESMA2012. Sponsors lecturers and mentors to the School.

- Center for High Performance Computing (CHPC), South Africa

CHPC makes available high performance computational resources over the network for School participants, particularly those who do not have access to adequate resources at their home institutions.

- Moi University, Eldoret, Kenya

Local organisers of the 2012 School. Interface with Kenyan government funding agencies and secure sponsorships from Kenyan commerce and industry.

| Project budget | | |
|--|--------------|---------|
| Amount requested from the ICSU Grants Programme: | | €30 000 |
| Estimated breakdown of cost | | |
| Research / Content | € 10 000 | |
| Travel / Accommodation for Meetings | € 20 000 | |
| Training / Teaching | € | |
| Planning / Coordination | € | |
| Other (specify): | € | |
| | | |
| Amount provided by the applicants: IUPAP C13 | | €7000 |
| Amount provided from other sources (specify): | | €85 000 |
| International Centre for Theoretical Physics (ICTP) | €30 000 | |
| IOM/CNR Democritos, | 3 flight tkt | |
| International Centre for Materials Research (ICMR), | \$35 000 | |
| USA IUPAP Liaison Committee, | \$6 000 | |
| Division of Computational Physics of the American Phys. Society | \$4 000 | |
| Beijing Computational Science Research Center | \$10 000 | |
| South African National Institute of Theoretical Physics (NITheP) | \$18 800 | |
| ICSU Regional Office of Africa | in kind | |
| Chepkoilel University College, Moi University | tba | |
| National Council for Science and Technology, Kenya | tba | |

Please provide a brief summary (300 words) of the project. This will be published in the ICSU website, should a grant be awarded.

- Project Summary

The African biennial School series on Electronic Structure Methods and Applications (ASESMA) aims to strengthen the field of computational material science in Africa by focussing on the fundamentals of the theory, algorithms and computation for properties of materials of great interest in Africa. The aim is to develop further the predictive power of materials computation in Africa. The School involves doctoral students and young researchers, and includes educational opportunities, and provides international-quality mentorships for research projects on a range of research problems in computational material science. This endeavour has the potential to add economic value to development of energy resources, minerals and materials relevant to Africa. The School has a strong pedagogical component, which develops the field of computational material science, and impacts on other cognate disciplines such as mathematics, physics, chemistry, material science, and computation, and in areas of the mainstream economy, with significant impact on the African continent. An important objective is to enhance intra-African contacts, networking and collaborations, and to create critical mass in a research endeavour that is amenable to rapid growth in Africa with the availability of cheaper computing resources, increasing bandwidth for African scientists, and the growing access to freeware codes such as the Quantum Espresso Codes. It is anticipated that there will be increased quality in graduate student supervision, and significant impact on quality research outputs as measured by publications in international journals and presentations at international conferences by African scientists. The 2010 ASESMA School took place in Cape Town South Africa, and the 2012 School will take place in Eldoret, Kenya. This ICSU grant is especially targeted at achieving the networking and collaborations for the two year period between the 2012 and 2014 ASESMA Schools.

APPENDIX

REPORT

African School on Electronic Structure Methods and Applications (ASESMA) Muizenberg, Cape Town 19- 30 July 2010. The inaugural school in the biennial series planned for 2010-2020

Summary of the ongoing activities of ASESMA

ASESMA-2010 was not just a two week school. It was the start of an ongoing network for interaction and collaboration. By all accounts, it was a fantastic success. The participants are continuing to stay in touch in 2011 long after the school. Several have started studies made possible by contacts made at the school, and there is enthusiasm for the future, and several others have gone to meetings in Europe through contacts made at the school.

* Much of the success of the school was due to an innovative program of mentors. The mentors are motivated young scientists mainly at the post-doctoral level, who worked with the participants one-on-one throughout the school. Since the school they have contacted every student; have on-going email communications advising on science and computing issues; set up web pages, a monthly electronic newsletter, and a Facebook page. (Links are given below). The participants, mentors and lecturers are enthused and the test will be the extent to which the interactions and collaborations continue into the future.

* The 2010 school was made possible by support of many international agencies:

* Support by the **International Union of Pure and Applied Physics (IUPAP)**, especially C13 and C20 commissions was essential for international recognition of the series and for financial support of the 2010 School.

* A key role was played by the **International Centre for Theoretical Physics (ICTP) in Trieste**. Without their financial support the school could not have occurred. Probably more important were the scientists from Trieste, the ICTP, **Democratis Italian Simulation Center**, for their tremendous efforts at facilitating the use and easy access of the excellent Quantum Espresso codes, for making these freely available, and for coordinating the lectures.

* The South African Institute of Physics provided financial and administrative support. Further sponsors included The National Institute for Theoretical Physics in South Africa, the SA National Research Foundation, The Division of Computational Physics of the American Physical Society, and the Materials Computation Centre at the University of Illinois. The University of Witwatersrand offered a bursary for postgraduate studies at its Centre of Excellence in Strong Materials to the best performing participant at the School.

* The mentors were funded by the **International Center for Materials Research (ICMR) in Santa Barbara** with strong support by Prof. Nicola Spaldin. The mentor program was the innovation that helped students on a one-on-one basis. This helped improve the pace of the delivery as the participants were able to work independently. Each participant was able to progress based on his/her own abilities.

* There has been significant international coverage of the school and series including:

A commentary published in Nature Physics, 6, 1 (2010). A copy is available at:
<https://netfiles.uiuc.edu/rmartin/www/2010-ASESMA-Nature-Phys-nphys1842.pdf>

A report in Physics Today – “Raising the scientific level and networking in Africa”, by Toni Feder. Phys. Today 64, 28 (2011) A copy is available at:

<https://netfiles.uiuc.edu/rmartin/www/Phys-Today-ASESMA-PTO000028.pdf>

* A description of the ASESMA series can be found at <https://netfiles.uiuc.edu/rmartin/www/AfricanSchoolSeries-rev-7-6.pdf>
This includes the international advisory board that consists of outstanding scientists.

* The websites and groups for ASESMA:

<http://asesma.ictp.it>

* A facebook page has been established

<http://www.facebook.com/?ref=logo#!/group.php?gid=145558648789192>

* A portrait gallery with contact information has been created.

<https://sites.google.com/site/asesma2010/>

* The 2012 school will be held at Moi University, Eldoret, Kenya, organized by George Amolo and Nicholas Makau. Efforts are underway to obtain support for participants and lecturers. IUPAP has committed to sponsor the series but financial support must be requested for each school. The ICTP has committed support for the 2012 school.

Report on the 2010 School in Muizenberg, Cape Town 19- 30 July 2010.

* Directors: Nithaya Chetty (University of Pretoria, South Africa), Richard Martin (University of Illinois, USA)

Sandro Scandolo (International Centre for Theoretical Physics, Trieste, Italy)

Lecturers: Stefano deGironcoli, Paolo Giannozzi, Nicola Marzari, Shobhana Narasimhan, Renata Wentzcovitch, Phuti Ngoepe

Mentors: Tesfaye Abteu, Kris Delaney, Sinead Griffin, Allison Hatt, Amy Lazicki, Brice Malonda

* At the 2010 School there were 45 participants (in addition to the 6 mentors) from many countries in Africa: Cameroon, Congo, Ghana, Ethiopia, Kenya, Nigeria, South Africa and Zimbabwe. Many of the South African students were actually nationals from other African countries, so the school served a large number of graduate students and young faculty. (See photograph below.)

* The School schedule can be found at <http://users.aims.ac.za/~sandro/>, which includes a link to the School photos.

* The topic of the Series of Schools is theory and computational methods for predicting and understanding properties of materials through calculations at the fundamental level of electronic structure. This is a growing field in which scientists with limited resources can have a large impact. A personal workstation is sufficient for many problems and the internet is making possible productive use of large computational facilities. It is within reach to create electronic structure community in Africa working at the level of forefront international research.

* The content of the 2010 School was a combination of theoretical background and hands-on calculations using workstations. Each student learned to install and use Linux codes, and the primary code for calculations was Quantum Espresso. Every student ran a calculation at the Centre for High Performance Computing in Cape Town, a facility meant for all Africans. A great effort was made to have coordinated talks on theory, computation, and on a phase transitions under pressure, a not-so-simple example of problems in minerals and geophysics.

The CHPC management invited each participant to apply for a user account which they can use from their home countries.

* The Centre for High Performance Computing in Cape Town has given all participants of the School access to their Blue Gene, which was donated by the IBM for African collaborations. The QE computations and collaborations could well be the first truly African-wide research activity on this facility.

* The African Institute for Mathematical Sciences (AIMS) provided a fantastic venue and backdrop for the hosting for ASESMA2010. The accommodation, catering, lecturing and computing facilities are excellent. For your information, the Canadian government has recently donated Can\$20m for the establishment of a network of AIMS centres in Africa that will include Ghana, Nigeria, Senegal, Ethiopia and South Africa, which is excellent news.

* There was excellent administrative support for the School by Milena Poropat (ICTP) and Linette White (South African Institute of Physics).

Richard Martin
Nithaya Chetty
Sandro Scandolo

Photograph of the participants, mentors and lecturers:





Regional Office for Africa

28 November 2011

Ms Rohini RAO
International Council for Science (ICSU)
5 Rue Auguste Vacquerie
75016 Paris
France

Subject: Support for ICSU Grant Application by the International Union of Pure and Applied Physics

Dear Rohini,

The ICSU Regional Office for Africa (ICSU ROA) hereby lends its support to the International Union of Pure and Applied Physics (IUPAP) for the project proposal titled "*African School of Electronic Structure Methods and Applications*".

In order to strengthen international science for the benefit of society, ICSU ROA encourages all efforts that aim at identifying and addressing critical disciplines on the continent, especially, like this one that focuses on strengthening the field of computational science and research in Africa targeting mainly young scientists and women scientists from within the continent. The proposed project will go a long way in creating strong science networks in the region, linking up scientists from the region with those from the other regions of the globe as well as in promoting collaborative research and mobility of African scientists and scholars in the region; an endeavour that fits into ICSU ROA activities of creating networks of excellence and human capacity building on the continent. As the theme for the 2012 African School of Electronic Structure Methods and Applications will be materials for energy, the output from this exercise will be useful in the implementation of ICSU ROA's existing sustainable energy projects as well as in the development of new ones.

ICSU ROA will be happy to be a partner in this initiative where it will play a pivotal role of providing guidance in identifying experts and scientists from the region who will be involved in the implementation of this project. The Office will also facilitate and foster links between IUPAP and the already existing African national research and educational networks as well as providing guidelines for action agendas and rendering administrative support in organising the implementation of the project.

ICSU ROA, therefore, gives its full support to IUPAP's application for support from ICSU to fund this project. As part of its commitment to promote the activities of the ICSU family in Africa, the ICSU ROA will avail its staff for any service that may be required, within the limits of its capabilities, for the smooth implementation of the project.

Sincerely,

Edith Madela-Mntla
Director, ICSU Regional Office for Africa



the academy of sciences for the developing world

ICTP Campus – 34151 Trieste – Italy

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Dr. Sandro Scandolo
The Abdus Salam International Centre for Theoretical Physics (ICTP)
Strada Costiera 11
34014 Trieste
Italy

25 November 2011

Re: ASESMA-2012 School in Kenya

Dear Dr. Scandolo,

Further to our earlier correspondence, I thank you once again for bringing to my attention the information about ASESMA-2012, the School that you are organizing in Kenya in 2012.

I am pleased to confirm the interest of TWAS to support this school. After consultation with the TWAS Programme Officer, Dr. Peter McGrath, the best option would have been to insert this School into the ICTP activities to be supported by TWAS in the framework of the institutional agreement between ICTP and TWAS for 2011/2012.

With best regards,

A handwritten signature in black ink, appearing to read 'R. Murenzi', written in a cursive style.

Romain Murenzi
TWAS Executive Director



Consiglio Nazionale delle Ricerche

Istituto Officina dei Materiali

Trieste, Cagliari, Grenoble, Perugia

To the organizers of the
African School on Electronic Structure
Methods and Applications (ASESMA)
Kenya 2012

Dear Dr. Scandolo,

I am delighted to continue the long-standing collaboration with ICTP in the organization of Schools on Electronic Structure Methods in different regions of the world (China 2004, Iran 2005, India 2006, Vietnam 2007, South Africa 2007, Chile 2009, South Africa 2010, Brazil 2011).

The DEMOCRITOS Simulation Center of CNR Istituto Officina dei Materiali is pleased to continue this tradition and to offer his support also for ASESMA-2012.

You can count on DEMOCRITOS for the following tasks:

- lectures on the advanced aspects of the theory and their implementation in the codes,
- coordination of the computational laboratories,
- making available the Quantum ESPRESSO code,
- technical expertise in the use of the codes.

I expect to be able to send three to four scientists from our Center to assist you in the above tasks. DEMOCRITOS may be able to cover the travel expenses of some of them, if the budget of the School was limited.

Sincerely,

Coordinator,
DEMOCRITOS Simulation Center
Istituto Officina dei Materiali
CNR

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