

5. Atomic & Molecular Physics Working Group

Stephane Kenmoe¹ and Obinna Abah²

¹Department of Theoretical Chemistry, University of Duisburg-Essen, 1654
Universitaetsstr. 5, Essen D-45141, Germany

²School of Mathematics, Statistics and Physics, Newcastle University, United
Kingdom.

5.1 Problematic

Atoms and molecules are the building blocks of matter. Together with light they are most of time indissociable entities. This stems from their fundamental quantum nature. Atoms as quantum particles are light. They can also be used to produce light that can be used for applications at the macroscopic level. Atomic and molecular physics (AMP) uses the properties of atoms and molecules to understand the properties of living and extinct organisms as well inert matter. AMP physics applications include a wide range of areas of technological relevance. These include biology, medicine, pharmacy, geology, electronics, spintronics, photonics, chemical industry, heterogeneous catalysis, cultural heritage, communications, security and many others.

However, probing matter at the atomic scale in Africa is a challenge. Both experimentally and theoretically. This stems from the various challenges of different nature. Among these, the main ones are the lack of experimental infrastructure, the scarcity of computational resources and resources limitation for efficient and large-scale capacity building. Recently, African scientists made important efforts to address these challenges. In this working group, we have assessed the challenges et opportunities for the further development of AMP physics at the continental level and report on the improvements observed during the recent years. Based on this assessment, we propose key recommendations that may help achieving research and education that align to local needs. This way we aim to contribute to rationalize the efforts needed for the development in AMP on the continent.

5.2 Working circumference

As a field within the framework of the African Strategy for Fundamental and Applied Physics (ASFAP), AMP namely through its applications is at the crosscut with many others: energy, computing and 4IR, astrophysics, biophysics, condensed matter and materials physics. However, in this chapter, we focus on the basic aspect of AMP. We concentrate on the basic requirements to enable efficient education and research, ongoing initiatives and perspectives.

5.3 Atomic and molecular physics in Africa: education and research landscape

5.3.1 A survey of atomic and molecular probes on the continent

Modern techniques for characterizing matter on the atomic and molecular scales are based on probe methods such as atomic force microscopy (AFM) or scanning tunneling microscopy, (STM) as well as spectroscopic approaches such as infrared Fourier transform (IRFT), vibrational frequencies sum generation spectroscopy (VFS) and various X-ray absorption spectroscopies (XAS) or fluoroscopy. Thanks to the latter, static or dynamic imaging of macroscopic objects with atomic resolution, or the minute working of dynamic processes such as attosecond-scale molecules decomposition in chemical reactions, are now possible.

However, the high cost of this equipment means that African scientists based on the continent have no chance of flourishing in this field. While access to advances in knowledge in this field is possible thanks to international collaborations and the growing popularity of open-access publications, the actual practice of experimental research is difficult, even in African countries that stand out for their greater investment in research, e.g. South Africa and Egypt. [1]

Apart from these two countries, for a many decades, capacity building on the continent has relied on continental initiatives like the African Laser Atomic Molecular and Optical Science Network (LAM). [2] However, over the years and in various parts of the continent, researchers have been able to set up national

laboratories with state to the art or low-cost instrumentation that allow to study matter at the atomic and molecular level and to perform research with potential applications in medicine, pharmacy, energy, light emitting devices, electronics and others.

The Atomic Molecular Spectroscopy and Applications Laboratory of the University of Tunis-El Manar: the pride of Tunisia

The laboratory is one of Tunisia's leading research centers, and its researchers have won international awards for their work on several occasions. Thanks to a wide range of laser-based spectroscopic methods, research in this laboratory covers many strategically important sectors, such as the environment, health, electronics and optoelectronics.[3] The laboratory has long invested in complementarity with theoretical research. This has given many sub-Saharan African researchers confined to the theoretical aspect of the field the opportunity to collaborate with local researchers.

Fluorescence Spectroscopy to study the impact of environmental conditions on herbal drug integrity in Ghana

Another focal point is the Laser and Fiber Optics Centre in Cape Coast University, Ghana, where fluorescence spectroscopy is used for herbal drugs characterization. The research at the Centre aims to be able to understand the impact of environment on the therapeutic properties and to make recommendations for herbal drugs storage conditions to maximize shelf life and preserve therapeutic efficacy [4].

Challenge for low-cost experimental physics in Cameroon

In Cameroon an initiative was launched a couple of years ago to face challenge of experimental physics. To this end, a biannual international conference on Low-Cost High-Level Physics and Solutions to real life problems was created. Periodic workshops are also organized and cover topics ranging from solar cells to optoelectronics, opto-mechanics, optical materials, nonlinear optics, optical telecommunications [5]. Besides, the so-called Challenge for Experimental Physics in Africa was launched in 2017 to encourage, mentor and promote

young scientists to design and build up inexpensive experimental instruments for daily life applications, e.g., in energy, environment, health....

A burst of pride in the Republic of Congo

Even in some favorable cases, where researchers have benefited from donations of equipment sent to their home countries at the end of their research stays in the northern hemisphere, follow-up or maintenance has often been lacking. It should be noted that the equipment in question is very often old-fashioned or slightly defective. A logical consequence of this is that the ambition to build a research laboratory with the help of these donations is generally not a long-lasting one. However, there are some rare cases worth mentioning. One of these is the donation of an AFM by the research center Elletra in Italy, which has led to the establishment of the first nanotechnology laboratory in the Republic of Congo in 2022. [6] If this is an encouraging start, aspects such as long-term capacity building are yet another credo.

The Africa Microscopy Initiative in South Africa

In line with previous initiatives such as “Imaging Africa”, the Africa Microscopy Initiative [7] aims to enlarge the African microscopy community, to provide world class infrastructure and training to African scientists so that the continent is not just a spectator of the evolution of knowledge, but also contributes to research, particularly in the medical field. The initiative launched by the University of Cape Town in collaboration with the Howard Hugues Medical Institute in the USA is designed to meet the pressing need for adequate resources to deal with local diseases. The instrumentation includes single molecule fluorescence microscope that allow to local illumination of sub-cellular organisms or proteins. At this stage, it has not been possible to draw up an inventory of the above-mentioned facilities on the continent. Even if they are available in some places, the striking reality is their scarcity. We still need more of such infrastructures and capacity building in the field!

5.3.2 Commendable efforts at the theoretical level

While experimental research relies heavily on collaborations with the rest of the world, considerable efforts are being made on the theoretical front, thanks to the development of synergies between researchers. The expansion of methods derived from quantum theory, such as the Nobel theory known as density functional theory, as well as recent advances in high-performance computing, have consolidated the bonds of collaborations. When we look at the poles of theoretical and computational research in atomic and molecular physics on the continent, it's clear to see that scientific production in the field is concentrated in North Africa, notably in Egypt, Tunisia, Algeria and Morocco, in Central Africa with Cameroon and the Republic of Congo, in East Africa with Kenya and Ethiopia and finally in South Africa. These countries offer a curriculum that one way or another includes atomic physics at least up to the masters level. Meanwhile in many other countries, this curriculum is missing.

Cameroon and Congo take the lead in sub-Saharan Africa

In Cameroon, several research groups have been working for several decades on the computational characterization of molecules with technological potential in optics, optoelectronics and nonlinear optics. Further north and south in the country, the products of the doctoral schools of institutions such as the Centre for Atomic Molecular Physics and Quantum Optics CEPAMOQ [8] in Douala and the different research groups University of Yaoundé (I) have been able to export their achievements and perpetuate the production of new knowledge, in the universities of Ngaoundere, Maroua and Buea.

Speaking of Buea, the impact of CEPAMOQ is resonant there. Several years after his training at CEPAMOQ, followed by a stay in Germany, a product of this center succeeded in setting up the University of Buea's Center for Drug Discovery (UB-CeDD), [9] precisely novel antiviral drugs inspired by compounds from African medicinal plants. Meanwhile it must be emphasized that the project is funded by institutions based out of the continent: the Alexander von Humboldt Foundation in Germany, and the Bill & Melinda Gates Foundation in the USA. The UB-CeDD aims to serving as a regional hub for the

discovery of new drugs in Africa, led by African researchers. The research combines virtual and in vitro screening techniques to identify natural compounds that target several vital proteins crucial for the survival of the HIV or SARS-CoV-2 viruses.

Meanwhile in Congo Brazzaville, a gradual shift from solid state physics to molecular surface physics has taken place in the last decade. Set up in the early days of CEPAMOQ, the School of Physics at Brazzaville's Marien Ngouabi University has gradually moved from the theoretical and computational characterization of bulk materials to the simulation of molecular reactions on catalytic supports. [10] The Catalysis and Magnetism Laboratory has been working for over a decade on surface molecular processes and their applications in catalysis, energetics and magnetism.

Nigeria and Ghana on track to do the same

At the federal University of agriculture of Abeokuta in Nigeria, the department of physics recently reshaped its research's landscape to include the investigation the properties of the leaves, bark, roots, and even of stems several plants for medicinal applications. [11] Using molecular dynamics simulations, the researchers at the department aim to provide a molecular level understanding of the biological activities the bio-organic compounds and hopefully aid in the identification of new therapeutic targets. Just to cite one example, the therapeutic potential of guava leaves is investigated for tropical diseases like malaria or typhoid. Similar projects are going on at the School of Physical Sciences, College of Agriculture and Natural sciences, University of Cape Coast in Ghana. [12]

5.3.3 Intra-continental synergies

It's worth noting the long-standing collaboration between the above-mentioned universities and South Africa: many researchers from sub-Saharan Africa have been able to find scientific asylum and forge collaborative links between their sister institutions. The fruits of these efforts are plain to see, with numerous publications to their credit. These include for example researchers from the

Cameroonian community and the University of the Free State [13]. At the same time, other members of the Cameroon of Atomic and Molecular Physics community have also forged links with North Africa, for example with the Laboratory of Atomic Molecular Spectroscopy of the University of Tunis El Manar in Tunisia, where several leading researchers from Central Africa have perfected a brilliant collaboration strategy that has resulted in several scientific publications [14]. These networks are distinguished by the mobility of talented researchers, who benefit from better research conditions, access to computing resources and therefore greater productivity.

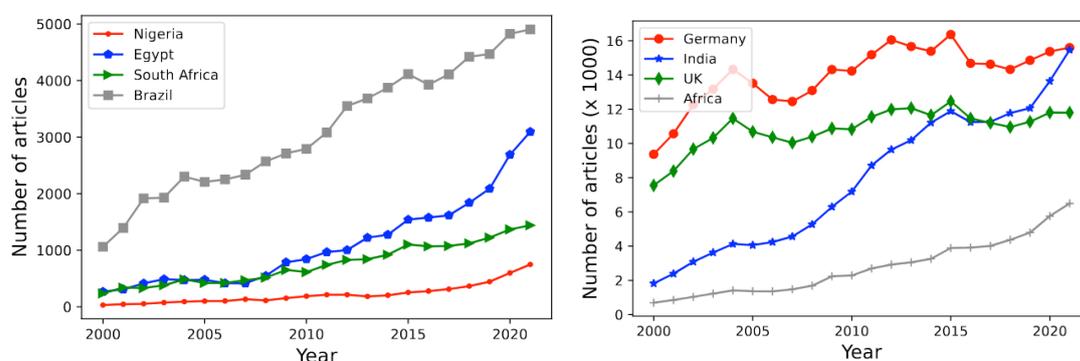


Figure 1: Research output per year from 2000–2021 for search keywords: atoms, atomic, molecular, molecules, or ions. (left) The number of articles published by some African countries (Egypt, Nigeria, South Africa) compared to Brazil. (right) The total articles published by African scientists (Algeria, Cameroon, Congo, Egypt, Ethiopia, Ghana, Kenya, Morocco, Nigeria, South Africa, Tunisia) compared western countries (Germany and UK) and India.

Source: Scopus – accessed October 8, 2022.[15]

5.3.4 Capacity building: regional and continental initiatives

Recently capacity building in electronic structure methods has led many research and networking opportunities within Africa and between African scientists and many hosts institutions around the world. The biennial African school on Electronic Structure methods and Applications (ASESMA) [16] and its regional schools held in Nigeria, Kenya, Ghana or Cameroon have contributed to strengthen the skills of young researchers on the continent. After 14 years of existence, hundreds of young African scientists have been trained

and initiated to the field of research. Through the ASESNET network [17], mobility and collaboration have been made possible between young participants and senior hosts both on the African continent and in the rest of the world. However, given the network's limited financial resources, other means of mobility and knowledge sharing need to be made possible.

The CASESMA initiative as a remarkable multiplier

The central African school on Electronic Structure methods and Applications (CASESMA) particularly has shone by its regularity since its inaugural event in 2018 and by the mobility opportunities within and outside Africa for the participants upon the school. [18] Dozens of collaborative research works within the participants have been published with the computing and open access support of the University of Duisburg-Essen. While CASESMA stands out by its regularity and sustainability in central Africa, other regional schools have not been taken place over many years. Young participants from outside Central Africa often attend CASESMA but in limited number due to the costs related their transportation which is most of the time as expensive as intercontinental travelling.

The pivotal role of CEPAMOQ in Douala, Cameroon

In Central Africa, and particularly in Cameroon, CEPAMOQ, based on the Cameroonian coast, has played a pivotal role in the implementation of atomic and molecular theories and their applications in optics, not only in Cameroon but throughout Central Africa. A few young researchers from neighboring countries such as Chad, Gabon, the Central African Republic and the Republic of Congo have benefited from further training in this field and are now setting up research groups in their respective countries, despite logistical and staffing difficulties. In recent years, Chad and the Central African Republic have seen the first batch of PhDs in this field trained at CEPAMOQ [19]. More regional centers like this are needed.

5.3.5 Supercomputers and High-performance computing in sub-Saharan Africa: an imperative need

One glaring aspect is the lack of computing resources. Researchers are dependent on the regional computing centers, thus making effective research impossible. Some in central Africa compute on the CEPAMQ clusters but most sub-Saharan scientists depend on South African universities, which in some cases offer free computing slots on their supercomputers. In addition to these barriers, the frequent power blackouts in the sub-regions are a serious hindrance, even when access to the computer is possible. It's high time that this part of the continent, if not every country in the region, acquires a supercomputer for the benefit of researchers and, above all, for research better aligned with local needs. At a time in contemporary history when the race to supercomputers is reaching cruising speed, when quantum computers are making computing power counters go wild and, above all, when artificial intelligence is becoming increasingly inseparable from computational data processing, it's inconceivable that Africa, and in particular the sub-Saharan region, is not in step with this major transformation not only of science but also of society at the global level !

5.4 Call for action: recommendations

If commendable initiatives can be observed, a question remains: do we want to do competitive research with the rest of the world or do we just want to survive? Should Africa always connote with poverty or low-cost means or do we want to show some ambitious? The latter is the goal of this strategy and there is an urgent need to act.

From what precedes, it is obvious that experimental research and education is more developed in Southern Africa and in Nord Africa. Sub-Saharan Africa still needs to improve with experimental research facilities. To palliate the lack of equipment, theory has emerged as what is seen by many as an alternative. However, as interdisciplinary and complementary scientists augur most often fascinating discoveries, it is high moon for this part of the continent to catch up with experimentation. With the critical mass of theoreticians and computational

scientists which formed over the recent years, it could soon be this critical moment when fundamental science followed by applied science could lead to technology aligned to local need and subsequently to prosperous economy and social progress. For this, we found the following items to be recommendable:

1. More regional centers like CEPAMOQ or the UB-CeDD as well as more frequent capacity building initiatives like CASESMA in other regions are needed.
2. Replicate the Tunisian AMOP laboratory and implement its model of collaboration throughout the continent.
3. Experimental facilities: STM, AFM, FTIR, spectrometers and other probes and capacity building for instrument usage.
4. Supercomputers & high-performance computing centers: high peak density in South Africa. Each region should have at least one computing infrastructure.
5. Promote complementary research particularly in sub-Saharan Africa to rationalize experimental research
6. Establish Collaborative Research Centers (CRC) e.g. via transregional research projects between theoretical centers in Cameroon and experimental groups in Ghana.
7. Align research to local needs: earth abundant hard and soft matter: heterogeneous catalytic supports, plants, dyes and others chemical compounds relevant for health, pharmaceutical chemistry, agriculture or energy.
8. Promote locally funded research via tax incentives: this will allow making good use of the young scientists trained during regional and continental events and limit the brain drain.

References