THE
AFRICAN PHYSICS
NEWSLETTER

James Sifuna and Javier Junquera

A tale of success

Javier Junquera, Professor Titular de Universidad, Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Facultad de Ciencias, Universidad de Cantabria, Spain

In July 2018, the University of Cantabria (UC) in Spain (http://www.unican.es) launched an open call to nationals from African countries to perform research in Computational Material Science. The grant awardee would be hosted by the UC Research Group in Theoretical Condensed Matter Physics led by Dr. Javier Junquera, with the funding provided by that group, together with the Vice-Rectorate for Internationalisation and Cooperation. The grant consists of a scholarship of EUR 10 000 to cover travel costs from and to the country of origin, living expenses and private medical insurance costs. The duration of the research stay would be of 10 months, divided in two 5-month periods.

After an exhaustive evaluation of applications including the CV, the motivation, and the overlap of interests between the African and the hosting group, the grant was awarded to James Sifuna, from the Technical University in Kenya. James is a Ph.D. student under the supervision of Dr. George Amolo and Dr. George Manyali from Masinde Muliro University of Science and Technology. This group is actively involved in the African School on Electronic Structure Methods and Applications initiative (ASESMA).

James has finished the first period, and the experience cannot be more positive. He has learned how to compile and maintain codes to carry out first-principles material simulations, using equipment from laptops to high-performance computing clusters (such as the Centre for High-Performance Computing in South Africa). Under the supervision of the hosting group, he has also learned the most important approximations, from the pseudopotential theory (including generation and testing) to the use of different basis sets (plane wave, numerical atomic orbitals, and tight binding), passing through the different flavors of density functional theory (including explicit methods to account for strong correlation), and the spin-orbit interactions. The goal is that the programs will not be used as black boxes, but instead will be settled on the well-established knowledge acquired.

James has carried out simulations on complex systems, such as the emergent metallicity at the head-to-head and tail-to-tail domain walls in ferroelectrics and the band structure of topological insulators like WSe2.

The second period, starting in January 2020, will be devoted to the study of optical, conductivity and thermoelectric properties of SrTiO3/SrIrO3 superlattices.

Overall, the initiative can be considered a complete success, with forward-looking prospects if allowed by future funding.