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Report back on the visit to Missouri University of Science and Technology, Rolla campus.

Project title: Nanodiamonds for solar cells applications

Investigators:

Principal investigator, UWC: Prof. Sylvain Halindintwali, Department of Physics and Astronomy

Co-investigator, UWC: Prof. CJ Arendse, Department of Physics and Astronomy

Principal investigator, Missouri: Prof. Vadym Mochalin, Department of Chemistry and Department of Materials Science & Engineering, Missouri University of Science and Technology

Time and duration of the visit: from the 1st March 2023 to 30th March 2023

I. What were the objectives of the visit?

The objective of the visit was to get acquainted with the synthesis, purification, and modification of the nanodiamonds (NDs) and explore their use as seeds for diamond thin film deposition in the existing CVD set-up in the department of Physics and Astronomy at UWC.

What was achieved during the visit?

On arrival in Missouri, the Missouri PI had purified NDs powder in his laboratory; we have used it to prepare NDs colloidal solutions within DMSO and DMSO/Methanol solvents. Using both centrifugation and direct & indirect sonication, we were able to get stable and well dispersed NDs solutions that we brought back in South Africa for future use. Preliminary characterization on the prepared solutions was done in Missouri using Raman spectroscopy in order to ascertain the presence of the diamond phase in the samples, and a Zetasizer Nano ZS instrument in order to determine the size of polydispersed ND particles in the solutions.



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II. How will your visit contribute to strengthening and improving your research / teaching at UWC?

The PI on the Missouri side subsequently visited UWC for two weeks at the end of April – beginning May 2023; the three investigators listed above identified four experiments that will be part of our collaborative research activities in the short term; a copy of a document detailing the four experiments is annexed to this report. The second listed experiment (b)) is already underway.

During his stay at UWC, Prof. V. Mochalin taught a condensed DFT (Density functional theory) modelling course to the MSc students in Nanophysics; he gave also an invited seminar/lecture to staff members and postgraduate students in the departments of Physics & Astronomy as well as of Chemistry, on Nanodiamond and MXenes – Fundamentals and Applications.

The proposed experiments on NDs and on the new class two dimensional MXenes – materials will be pursued and the outcomes will be made known later. On the teaching side, we aim to invite Prof. V. Mochalin for another series of lectures next year.

III. What are your future goals, following this mobility?

The future goals, following this mobility would be to use the NDs as seed layer for further growth stoichiometric SiC layers and diamond like materials. We will also introduce the NDs in perovskite solar cells for possible improvement in mechanical properties and /or improved photons absorption. Oxidized MXenes materials will be also incorporated in perovskite solar cells for possible improvement in optical properties. This is a good opportunity for postgraduate students to work on these cross-cutting new fields. Once we have evidence of the sustainability of our collaboration (the results of the proposed experiments as measurable indicators), we will work on joint applications for funding.

IV. To what do you ascribe your success and challenges?

The challenges we experience so far are ascribed to loadshedding (revolving electric power cuts in South Africa); we are currently unable to schedule experiments requiring high vacuums and extended times of processing; in the meantime, we are exploring and optimizing the spin-coating route that does not require extended periods in synthesis and at the same time it is a low power intensive technique. The project on diamond-like and SiC materials may be on hold for a while until we have a reliable power backup for our cvd laboratory and/or the power grid will improve.



Department of Physics & Astronomy



V. How do you locate the value of the UM / UWC Exchange Programme within the goals of your department / faculty and subsequent work?

Although it was my first time to travel to Missouri, many other colleagues from the department and from the faculty have been there previously and they have established long lasting and sustainable collaboration with the Missouri partners. The UWC co-investigator on this project is a very good example. We will draw from his positive experiences to advance this new project. The first positive outcome is that the PI on the Missouri side has already promised the availability of his characterisation setups for measurement techniques not readily available at UWC.

VI. What changes and improvements do you recommend?

As I was traveling for the 1st time to Rolla / Missouri to discuss the feasibility and launch a new project, it would have been more interesting to have some kind of transport in order to explore the beauty of the place in my spare time outside of the university premises. Unfortunately, I found the public transport system limited in the city as well. My recommendation is to provide staff members visiting Rolla with a transport in order to allow them to access the shops and other touristic places.

VII. What has been the most rewarding about the programme?

Besides the lab work related to my proposed project, I was able to attend a series of seminars that are a regular feature in the faculty I visited; we can learn a lot from them if we aspire to be a vibrant faculty where knowledge and results are shared on a regular basis.

I appreciated the warmth of the hospitality I received from the host PI in Missouri; it was also rewarding that he accepted our invitation to visit UWC as well.

Acknowledgement

We are grateful to the University of Missouri - University of the Western Cape Academic Exchange Programme to have accepted to fund this project. We acknowledge also the guidance of Prof. Rodney J. Uphoff, Director, UMSAEP & Elwood Thomas, and his proficiency in organizing all the required paperwork.

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