DR GUGU KHUBEKA

PROJECT: Modelling of Fluorinated Transition Metal Oxides for Application as Energy Materials in Flexible Solar Panels

Background and Rationale

Renewable energy sources, such as wind, hydro, solar, hydrogen and bio, are free of pollution and afford great relief from the global warming threat posed by the excessive burning of fossil fuels (e.g., coal, oil, and gas). Solar energy is the most abundant of all energy resources for heat, light, and electricity generation, through thermal power generators and solar cells.

This technology is clean and green and produces no greenhouse effect on the environment. Furthermore, the current energy markets are moving towards the use of green energy systems and solar panels form an integral part of such green energy technologies.

Despite all these benefits - because of high manufacturing and installation cost - the use of solar technology for power generation is only 1% of the energy market. Therefore, there is still a need to design and develop low-cost and efficient energy materials to help lower clean energy costs. Research has shown that transition metal oxides, in a fluorinated form, present some of the most high-performance energy materials in the world. Tin oxide, in particular, has a huge market value, and its fluorinated form is used in electronic displays and as transparent electrode material in flexible solar panels.

Using molecular modelling techniques to predict the properties of such fluorinated transition metal oxide materials is crucial for research and development, primarily since it lowers research material costs and increases the power of simulation. This increases the ability to predict various structural designs and effectively narrows the pool of the desired final product structures and physical properties prior to actual laboratory tests and subsequent manufacturing.

The application of models to simulate experiments on energy materials is becoming increasingly useful, providing invaluable data for potential alternative candidates in material development.

The South African Nuclear Energy Corporation (Necsa) has the technology to model and synthesise fluorinated materials for application as energy materials in solar panels.

Objectives and methodology

The first strand of my research is to model different structures of fluorinated SnO2 (FTO), using molecular modelling. The aim is to identify structures that are most stable, can harness more solar energy for efficient energy production and are cost-effective in terms of production. Research in the area of SnO2 and other related metal oxides requires modelling capability to predict material properties and the ability to carry out fluorination to bring to life the simulated scenarios.

- DFT calculations using Vienna Ab initio Simulation Package (VASP) and Phonon will be performed to gain insight into electronic and vibrational properties of SnO2 and FTO.
- The second strand of this research will involve laboratory-scale synthesis of the identified potential energy material candidate from the simulations. The focus here will be to develop new and low-cost synthetic pathways which could result in a patent.
- Low temperatures and cost-effective techniques such as hybrid sol-gel, chemical vapour deposition, and hydrothermal will be employed.
- The third strand of this research will involve testing and applying the materials as flexible solar panel components.
- Optical and electronic properties will be studied using various instruments
- The fourth strand of the research is to ensure that the products have commercialization potential in energy space, where solar panels are applied.

Timeline

The research activities will be divided into four work packages (WP) over a period of three years:

WP1- Molecular modelling will be done using MedeA mini-computer cluster equipped with VASP and Phonon simulation packages.

Timeline: Years 1 and 2

WP2 and WP3- development of new synthetic routes and improving electronic properties. Small-scale experiments to fluorinate SnO_2 will be done, using thermogravimetric equipment and small laboratory-scale reactor. The data will be profiled to choose the candidates with better results. Infrared, Raman, and UV-vis spectroscopy, Thermogravimetry, Powder X-rays and Neutron diffraction will be employed to study the structure and electronic properties of the newly developed materials.

Timeline: Years 1 and 3

WP4-Commercialisation/patent: the plan is to develop alternative and unique ways to produce these materials so that Necsa can have the freedom to operate. The products have commercialization potential in the energy space, where solar panels are applied. The products are also used in space technology, like small cube satellites built in Stellenbosch University, on their flexible solar panels.

Timeline: Year 3

Results or preliminary data

Based on molecular modelling calculations, the material with ideal properties for application in solar panels must form stable nanostructures given by the Vienna Ab initio Simulation Package (VASP) energy. Different defects on the SnO_2 structure have been modelled and the stable structure has been identified. Introducing defects enhances the optical and electronic properties of SnO_2. The improved optical and electronic properties include wide absorption spectrum, high conductivity, ≈100% transmittance to visible light, low toxicity before and after production as well as high thermal stability. Furthermore, the low deposition and low temperature techniques were successfully chosen to produce these materials.