Solid State Luminescent and Advanced Materials

The main projects are:

Solid State Luminescent Materials

The main objective of the research associated with the Research Chair is to develop micro- and nanophosphors for applications in infrastructure and high technology flat panel displays. The fabrication and the test of these phosphors, which have a long after glow, for infrastructure development, and phosphors which will withstand degradation, for flat panel display applications, will be the main challenge. Nanotechnology will provide tools for high tech development as well as development in rural areas. The fabrication of phosphors will provide affordable lighting for people in rural areas, assisting with national infrastructure development, but may also be used in high technology plasma and field emission television screens. The main aim of this research area is to push the frontiers of knowledge within or between disciplines and to ensure recognition, both nationally and internationally, of the high quality of the research. Specifically, the development of nanophosphors which may be excited with rays from the sun during the day and then brought into the house at night, giving light to read and study, is one example of how this research may assist in reducing vulnerability and contribute to poverty alleviation, this will be done in collaboration with the CSIR nanogroup. Nanotechnology development will help South Africa to compete internationally, bring about new innovations, take South Africa to a higher level of science and engineering and will also help build capacity in technology human resources and transformation Organic electroluminescent (EL) devices have attracted significant attention due to their promising applications in solid-state lighting and full-color flat-panel displays. OLEDs used in lighting applications are expected to become very popular in the next few years and will initially target niche markets; the technology has several advantages over that of conventional lighting. First among the advantages is slimness. The thickness of OLED panels for lighting applications could reach less than 1 mm. The flexibility is another advantage, which may allow OLED lighting to be used when designing for limited spaces. Different methods are used to obtain white organic light emitting devices (WOLEDs). One is the mixture of the three prime colour phosphors, red, green and blue. The main challenges are still to obtain high-resolution patterning of EL devices and to reduce fabrication costs. The active layers of organic light emitting diodes are commonly fabricated by spin-coating, vacuum deposition and ink-jet printing. Tris-(8-hydroxy-quinoline) aluminium (Alq3) has been used in OLEDs both as a green light emitting material and as an electron transporting layer (ETL). OLEDs consist of an EL medium of thin layers (<0.2 μm) sandwiched between two electrodes. Some organic layers transport holes and others electrons. When a potential difference is applied between the anode and the cathode the holes and electrons will migrate toward the opposite charged electrode. Holes and electrons then transfer to the emitting material forming tightly bound excitons which emit a photon upon relaxation. These photons are then capable of escaping the device architecture through the transparent anode and out the glass substrate.

Organic photovoltaic (OPV) devices made from a blend of conjugated polymers have attracted much attention because of their promising improvement of power conversion efficiencies. Solar cells (photovoltaic (PV) materials) currently have very low energy efficiency and expensive manufacture costs are involved. The Shockley – Queisser limit for the amount of sunlight that gets converted to electricity is only about 30%. Most of the sunlight's (solar spectrum's) energy is therefore lost. Phosphor material may be used to absorb and to convert some of the lost energy to the solar cell in order to produce more electricity. There is a growing demand for energy and electricity production to about 10 billion people on earth. The vast majority of energy production is through combustion of fossil fuels. Alternative ways to provide cleaner and safer energy is mandatory because fossil fuels produce CO2. CO2 has a detrimental effect on the composition of the atmosphere, the global temperature, the sea levels and the weather patterns. Choosing the ideal phosphor for a specific solar cell has the potential to increase the energy efficiency. The phosphor material has the advantage that it can be added externally to any PV material without impacting the highly optimized solar cell designs. High efficiency solar cells require absorption of photons of the full solar spectrum and although this approach is still a long way from being practical it provides the best opportunity to truly increase all solar cells' efficiencies. This project therefore investigates how to combine phosphor material with solar cells for the maximum electricity production by using the down-conversion approach. Down-conversion is the quantum cutting of 1 high energy photon into 2 lower energy photons. This approach has not received much research attention yet. Efficient phosphors can be used as UV down-converting or Infra-red (IF) up-converting layers to improve the absorption efficiency and enhance general performance of the conventional silicon photovoltaic cells.

A theoretical and experimental study on the formation of Nano-particles

Creating nano-crystals is relatively easy, but creating nano-crystals with particular shapes and sizes is more difficult. To manipulate and control the shapes and sizes of nano-crystals, the physical and chemical properties involved during the growth/creation processes have to be understood clearly. However, little is known about the underlying elementary physical and chemical processes (on the atomic scale) during the formation of nano-crystals. This project will address this knowledge gap by studying the physical and chemical processes involved during the formation of nano-crystals.

The first objective is to develop a custom Molecular Dynamics (MD) software package to model the atomic interactions and movement on a surface. A small computer cluster for parallel computations will be setup for development and preliminary calculations. During the first phase the focus will be on some of the FCC metals (Al, Au, Ag, Cu, Ni, Pt). Once the MD software is operational, it would be converted to run on a High Performance Computing cluster (HPC) which will speed up the calculation speed and shorten the calculation time significantly. The second objective is to utilize the MD software to study the migration- and segregation of atoms migrating on a surface and in the bulk of large single crystals. These simulations will be compared with experimental segregation and migrating measurements to verify the accuracy of the simulation. The third objective will be to focus on simulating the growth of nano-particles during physical vapour deposition. The simulation will be compared with real nano-particles grown in a custom build physical vapour deposition system. The physical vapour deposition system will be designed and built in-house, especially for growing nano-particles on a surface for the vapour phase. The fourth objective of the project will be to focus on the behaviour of nano-particles during heat treatment. This will be done by studying the properties and physical behaviour of impurities in simulated nano-crystals, looking at the activation barriers and determining diffusion coefficients of surface-to-subsurface diffusion as well as activation energies for vacancy migration. (This is ambitious and challenging.)

Petrochemicals

The third focus area of petrochemicals includes thrusts in homogeneous and heterogeneous catalysis, which converts basic building blocks of the sub-/ lower-nanoscale size into value added downstream nanochemicals, relevant to the synthetic petrochemical industry. Catalysis is a vast and integrated part in many chemical conversions, dramatically increasing the rate of formation (of new compounds/ solvents/ detergents/ materials) as well as selectivity (specific characteristics) of tailor-made products. It requires clean operating systems from the onset from both economic and environmental considerations since the process is more effective to yield pure products with higher yields and minimising waste. It thus includes research which ensures minimal environmental impact in the pursuit of green chemistry. Aspects related to both Homogeneous and Heterogeneous catalysis will be explored in close collaboration with UFS Chemistry, utilising variations of middle to late transition elements to catalyse the reactions of interest (typically, oligometisation, hydroformylation and carbonylation reactions.)

Advanced Materials

Some of the involved UFS group members will investigate the hardness of a super alloy after the addition of nanomaterial precipitates and others will concentrate on the Kinetic Monte Carlo calculations describing the occurrence of processes during nanoparticle synthesis. For producing pre-painted coated material that is used for the manufacturing of domestic appliances (fridges etc), cool rooms (ZoZo huts), sign boards and roofing (Chromadek), the surfaces of materials need to be completely understood. The state of the art surface characterization equipment to our disposal puts us in an excellent position to characterize these surfaces.

Multidisciplinary research

Cross-cutting multidisciplinary research is one of the main focus areas of the chair in which Physics, Chemistry and Microbiology will form a strong synergy amongst them. Scanning Auger Microscopy (SAM) in conjunction with targeted Argon (Ar+) etching is usually used in the study of conductors and semi-conductors and has never before been mentioned in cell biology (especially yeast). However, in 2010 the use of this technique on biological material was reported for the first time by the Kock and Swart group. In this study the effect of fluconazole (an important drug in use today to combat yeast infections) on ascospore development in the yeast was demonstrated. These results lead to several other future projects in which yeast cells will be investigated. For the basic catalytic reactions, multidisciplinary research with UFS Chemistry group is also included.