Inaugural Lecture:

Computational Chemistry-the alternative to chemistry in a laboratory

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In the age of the 4th Industrial Revolution, the field of computational chemistry finds its place quite easily. This particular area of science makes use of computer simulations to find solutions to both old and new challenges, case in point, the current Covid-19 pandemic. Because of this mode of research we are able to dispense vaccines within a year that can help to curb the intensity of the virus when infecting people.

Figure 1 below describes how computational chemistry lends itself to experimentalists and its great advantage thereof going from desktop calculations into the laboratory.

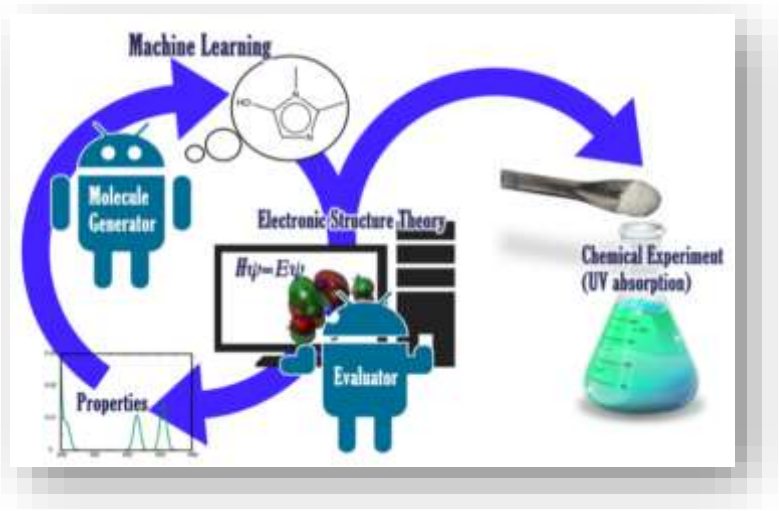


Figure 1: Theoretical and Experimental Chemistry working hand-in-hand

Computational Chemistry is beneficial on many levels and helps to promote greener chemistry, saves on chemical cost and time, attempts to solve problems that involves dangerous elements (which can't be done in a lab) can be explored and so much more.

Currently the world and South Africa is facing challenges in both the water and energy sector. We are using computational methods to try and address some of the challenges and help improve on the availability of water (a basic human need) and to increase the supply of energy which because the lack of we continue to experience days of load shedding.

Although water is abundantly available, not all of it is fit for human consumption therefore our focus is to look into waste water treatment and design suitable and economically viable materials that can easily assist in waste water treatment especially in poverty stricken areas.

One such pollutant contaminating water sources are organic dyes. The devastating effects of toxic organic dyes on human health and the environment have necessitated the need to devise holistic techniques for their effective removal of pollutants from water. Although semiconductor photocatalysis is deemed as a holistic method for eradication of dye pollutants from water, the technology is hindered by some inherent problems. These problems include their ultraviolet light

activity instead of visible light due to their wide band gap, and the fast recombination rate of the photogenerated holes and electrons.

Figure 2 below, provides a schematic on the photocatalysis mechanism that occurs in the presence of visible light.

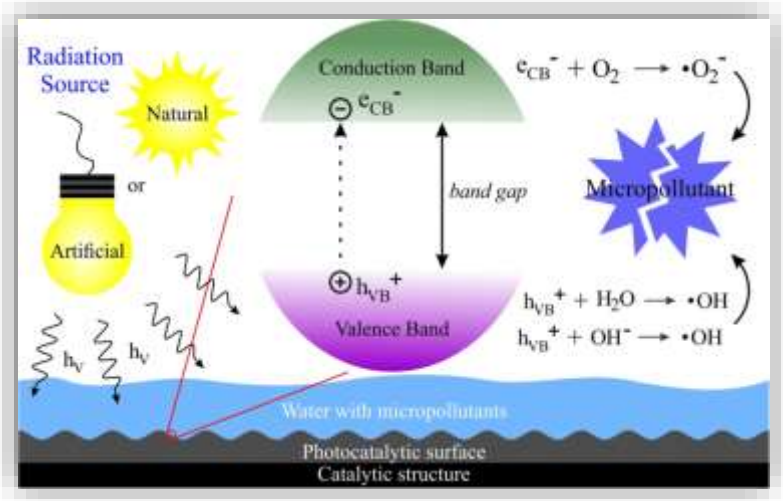


Figure 2: Mechanism of Photocatalysis

It is very important to design a material that can work in the visible range so that degradation of organic pollutants may be initiated and broken down into harmless chemicals. Therefore our research group places emphasis on the design of photocatalytic materials in order to assist with this process of decontaminating waste waters. So far we have worked on materials such as: multi-walled carbon nanotubes, La doped ZnO, Cubic $SrTiO_3$ with perovskite-type materials of the type, $MTaO_3$ (M=Na, K) and so forth.

For the perovskite-type materials, the $MTaO_3/SrTiO_3(010)$ heterostructure showed high photocatalytic activity under visible light irradiation with good stability and reduced bandgap compared to the bulk $SrTiO_3$. The heterostructures formed a type-II band alignment (Figure 3) to accelerate the interfacial charge transfer process and the photocatalytic activity.

By comparing the relative ratio of effective mass, we concluded that $MTaO_3/SrTiO_3(010)$ heterostructures has not only superior mobility of charge carriers, but also higher separation of photoinduced electrons and holes. The band alignment results showed that the $MTaO_3/SrTiO_3(010)$ heterostructures are highly efficient for pollutant degradation and energy conversion. In summary, this study showed a key role of $SrTiO_3$ as an electron donor to enhance the optical properties and stability of $MTaO_3/SrTiO_3(010)$ heterostructures.

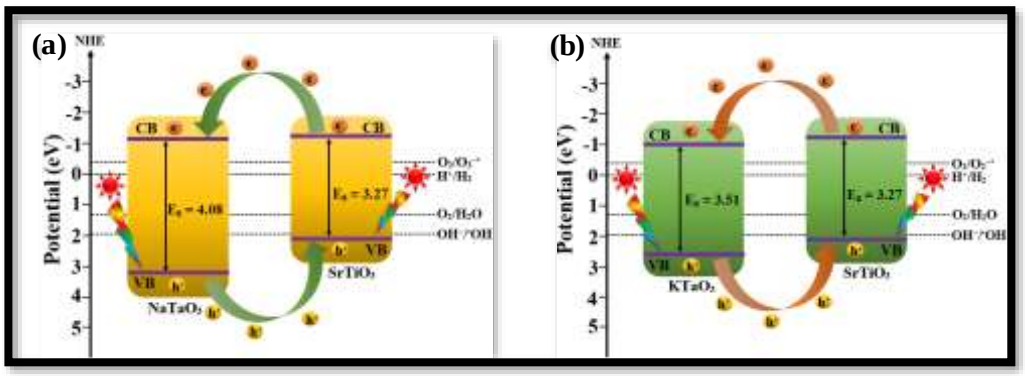
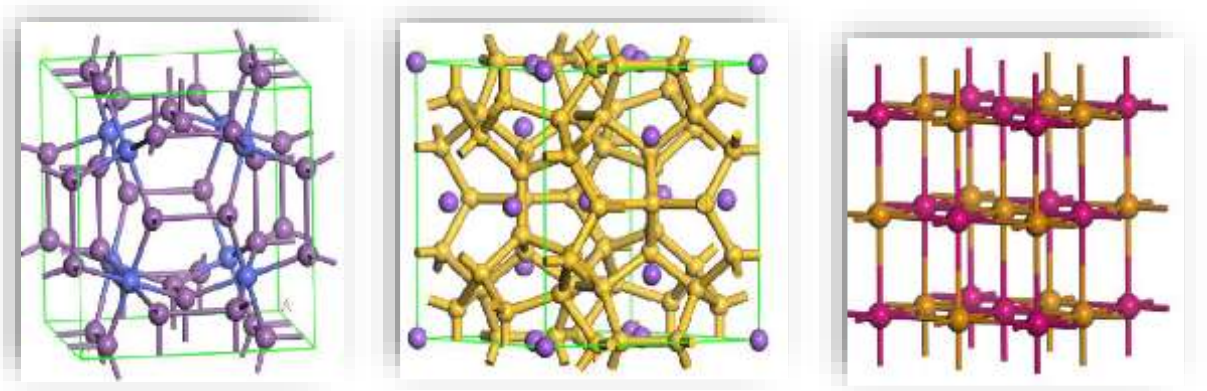


Figure 3: Photocatalytic Materials with band II alignment

On the other hand we have also looked into how we can explore areas of energy such as Thermoelectrics (TE). This is becoming an extremely important area of research as its one way in which we can maintain a sustainable form of energy for the future. Thermoelectrics can be defined as the conversion of heat energy into electrical energy. There is indeed a lot of wasted heat energy from current methods that make use of mechanically driven processes thus thermoelectrics is one such way to harness this energy for reuse.

So far we have computationally explored potential TE materials such as skutterudites, clathrates, 2D nanostructures such as transition metal chalcogenides and some carbonaceous materials (Figure 4). By investigating certain parameters of the materials such as: band structure, density of states (DOS), spin DOS, projected DOS, charge transfer, ionisation energy, electron affinity, electric potentials, absorbance, electrical conductivity, reflectivity, dielectric function and phonon dispersion we were able to monitor as to whether the electrical conductivity of the TE material increased while the thermal conductivity decreased. These are considered as ideal conditions for an efficient TE material.



$CoSb_3$ (skutterudite) | Na_8Si_{46} (Na_4Si_{23}) lattice clathrate) | $AgSbTe_2$ (chalcogenide)

Figure 4: Example of skutterudite, clathrate and chalcogenide

Our future outlook for these two research domains aims to move into making real products that can be bought economically and used to a maximum. It is in our best interest and that of the country to continue to find ways to ensure water, a basic human right, is made available to all people while also finding greener and better ways to also keep the lights on.