US-Africa Initiative Workshop

APS March Meeting - Sunday, March 14, 2021

Sponsored by the APS Innovation Fund

N.F. Andriambelaza

Postdoctoral Fellow

University of Pretoria

arinala.f@gmail.com

The main interests of our research group are based on the study of two dimensional (2D) graphene-like materials. I am a postdoctoral fellow in the group of Theoretical and Computational Solid State Physics under the supervision of Prof. Nithaya Chetty. At the moment, I am the only research fellow under his supervision at the University of Pretoria.

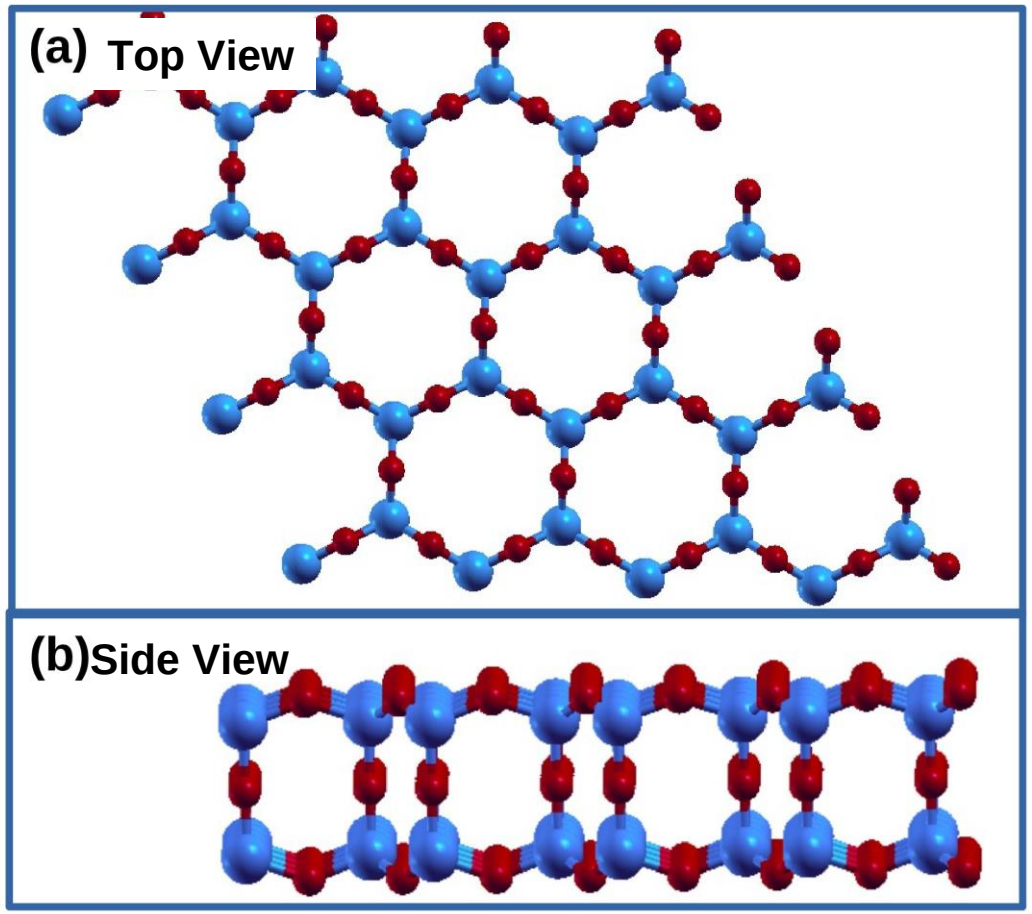
Density functional theory (DFT) embedded in the Quantum Espresso and Vienna Ab initio Simulation Packages are used in our group. We are mainly interested in the study of the stability, structural, electronic and catalytic properties of various 2D materials such as silica bilayer (2D zeolite model), transition metal dichalcogenides and oxides for nanotechnological and catalysis applications.

Creating complex systems such as introducing defects, adatoms and alloying can enhance the properties of the 2D materials and broaden their applications. Any collaboration related to these studies on 2D materials will be appreciated. The work is computationally expensive and access to powerful computers is required.

Some of my work on band gap engineering of MoS_2 monolayer can be found on the link: http://hdl.handle.net/2263/70608

Possible collaborative projects

2D zeolite model



1st project:

- First principles studies of P, N, As substituting Si in the 2D zeolite model. The stability, structural and electronic properties of the doped system will be investigated.
- Introduction of group I elements as charge compensation due to the introduction of pentavalent atom.
- How about if we introduce anions such as F, Cl, Br and I atoms?

2nd project:

First principles studies of Al substituting Si in the 2D zeolite model having noble metals such as Pd and Pt as charge compensation for catalysis applications.

3rd project:

Investigation of the physical and chemical properties of CO_2, TiO_2, GeO_2 and SnO_2 in silica bilayer-like structures.