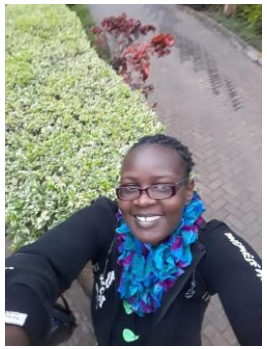
US-Africa Initiative
Workshop at APS March Meeting
Sunday, March 14, 2021

ab-initio Studies of Effects of Doping on Selected Titanium Oxides



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The objective of this work is to study the structural, electronic and optical properties of the higher oxide phases of Titania, such as Titanium Sesquioxide (Ti_2O_{2n-1} ,n=2) and it's oxynitrides ($Ti_nN_2O_{2n-3}$, n=2) in addition to the widely studied Titanium dioxide (TiO_2), as well as Titanium dioxide doped nitrogen (TiO_2:N), using DFT. We've looked at the structural and electronic properties of the oxides at DFT and DFT +U levels of theory.

However, we are still working on the optical properties of the oxides using many body perturbation theory with GW approximations as implemented in the yambo code. These require huge computational resources, the Centre of High-Performance Computing (CHPC) through the project MATS862, Rosebank Cape Town Republic of South Africa is appreciated for providing access to the HPC cluster facility used in this research. Much appreciation to my research supervisors, and Materials Modeling team at the Technical University of Kenya under the mentorship of Prof George Amolo.

Material Modeling Group, TU-K.
http://spas.tukenya.ac.ke/

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ab-initio Studies of Effects of Doping on Selected Titanium Oxides

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Problem Statement

Solar cells address the issues of (i) global warming as a result of combustion of fossil fuels, (ii) increase in global energy demand and (iii) depletion of fossil fuels. TiO_2 is used as an absorber layer in solar cells , it's photo-activity has been increased by incorporating other elements into it's structure. However, the possibility of doping the higher oxide phases of Titania has not been adequately explored.

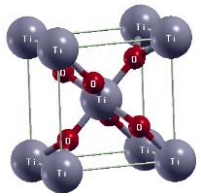
Objectives: To study the structural, electronic and optical properties of TiO_2, TiO_2 :N,Ti_2O_3 and Ti_2N_2O.

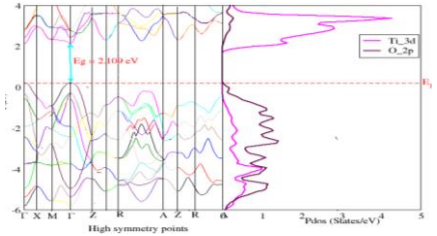
Methodology: All calculations were carried out using density-functional theory (DFT) as implemented in Quantum ESPRESSO computer code and yambo code..

Work in progress: Study of optical properties using yambo code.

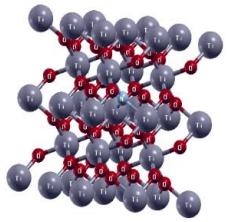
Preliminary Results and Discussions

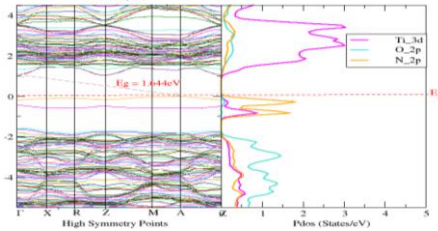
a)TiO_2



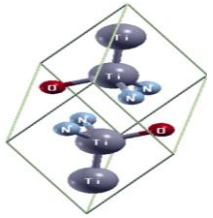


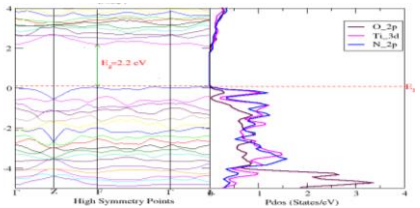
b)TiO_2:N





c)Ti_2N_2O





✓TiO_2:N has a reduced band gap compared to pristine TiO_2,.

✓In-gap states (acts as recombination centers) are observed in the TiO_2:N band structure as a result of N_2p impurity states.

✓Ti_2N_2O has a band gap of 2.2eV which is clearly near the middle of visible light and do not have in-gap states.

Conclusion

Ti_2N_2O is likely to be a more promising visible-light-driven material for photovoltaic applications compared to pristine TiO_2, TiO_2:N and Ti_2O_3.