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Bruno DANDOGBESSI

IMSP-BENIN, Lecturer,
bdandogbessi@gmail.com

My research is mainly devoted to computational quantum mechanical studies of materials especially renewable energy materials. I address electronic, structural, and transport properties from a fundamental perspective.

The methods that I used are density functional calculations, which are then fit to treat large systems. I've have a collaboration with solely the group of Dr Omololu Akin-Ojo. in the ICTP-EAIFR (University of Rwanda) who works in sustainable materials for energy. I also used Fortran code to analyze transport properties for models systems such as ratchet systems.

I apply theoretical and computational methods to predict and engineer material and molecular properties from first principles. I focus on relevant problems to the development of sustainable energy sources and quantum technologies.

Research Interests and Possible Collaborations

1)Properties of strongly correlated oxides and their applications
2) Materials Discovery for catalytic activity
3) Nanoparticles and nanoclusters
4) Engineering charge state on 2D surface (graphene & hexagonal boron-nitride) for catalytic activity
5) Water-metals interactions
6) Simulations methods development

My work require access to powerful computers. Thus I am looking forward to access the computational resources and in order to develop my knowledge and train more students. Of course the goal for future collaborations passes from some exchanges of knowledge and I am queen to learn how to use machine learning.
7) Possible Collaborations Prof Renata wentzcovitch & Prof Giulia Galli and others….