

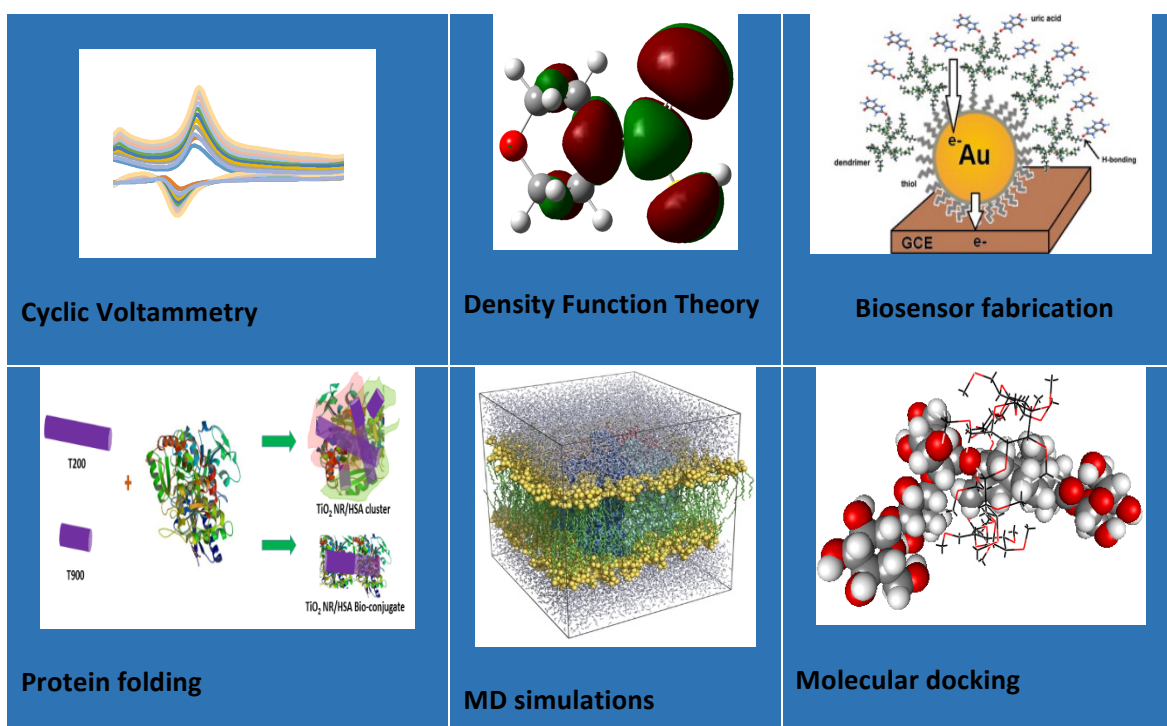
COMPUTATIONAL MODELLING & BIOANALYTICAL CHEMISTRY



The focus of our research is largely based on High Performance Computing (HPC) ranging from small organic molecules to bioactive macro-molecules. Our interest includes the development of computational models for the design of more effective host-guest systems using state-of-the-art molecular dynamics and docking simulations supported by experimental studies. In addition, our research also includes structural characterization and property prediction for molecules, materials, and biological polymeric compounds. The broader goals are to design, model and fabricate smart materials doped with nanomaterials to improve drug delivery systems and biosensor technology. The experimental techniques employed in this research ranges from electrochemistry, capillary electrophoresis through to thermal methods.

PROF K BISETTY (PRINCIPAL INVESTIGATOR)

CURRENT RESEARCH ACTIVITIES



GROUP MEMBERS:

Dr. S.Kanchi (Research Associate)
Dr. Deepali Sharma (PDF)

Doctoral students:

Mr. N.J. Gumede
Mr. M.I. Sabela
Mr. M.S. Shahbaaz

Masters students:

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Mrs. L. Ramsarup
Ms K Kuene
Mr K Balgobind
Mr Bayu Trimurthi
Ms Athika Putri

PAST STUDENTS:

DR P Singh (PDF)
Dr T Singh (masters)
Dr P Govender (masters)
Dr P Mokoena (PhD)
Dr P Sharma (PhD)
Dr. Faez Iqbal Khan (PhD)
Dr. B. Ayyappa (PhD)
Mr. N.J. Gumede (masters)
Mr. M.I. Sabela (masters)
Ms N Singh (masters)
Mrs. S. Khulu (masters)

COLLABORATORS:

1. Prof M Hassan, Center for Interdisciplinary Research in Basic Sciences, Jamia Millia Islamia, Jamia Nagar, **New Delhi**
2. Prof Mikhael Bechelany, University of Montpellier, **France**
3. Prof A Tiwari, Associate Professor Department of Physics, Chemistry and Biology (IFM), Linköping University, **Sweden**
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5. Prof JJ Perez, Barcelona, **Spain**