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Future Research Interest/Proposal

The computing technology is growing exponentially and changing the development activities of new materials. At present, the first principle calculation methods and programs are a powerful research tools, which enable the experimentalists to predict the structures and properties of a material or compound before its synthesis. On this theme two research proposals (based on first principle studies) are :

Proposal 1 : Tailoring the Graphene structured materials for NanoFET/BioFET

Bio-FETs have become one of the major technologies for detection of ions, DNA, proteins and other biomolecules. The working principle of Bio-FET is to monitor the conductance change in the gate channel, before and after the adsorption of target molecules. Due to its large sensing surface and excellent electronic properties, graphene, the principal 2D material, has attracted significant interest to use as a channel in FET sensors. Other graphene structured materials viz. stanene, ZnO nanoribbons, Transition metal dichalcogenides, have direct band gaps and excellent electronic properties, which offer gate-tunable conductance and make them attractive for FET sensor applications.

The aim of this proposal is to tailor 2D materials and investigate sensing performance of nanoFET/ bioFET under various physical conditions, structural geometry, layer of material and thickness/length of sensing 2D materials with and without doping/interaction of impurities/ biomolecules on the sensing surface. The work is planned as

Designing, structural and stability analysis of 2D sensing surface and electrodes.
Mechanical strength, electronic and optical properties study with different physical conditions.
Designing of nanoFET/BioFETs and their I-V characteristics analysis with and without doping/interaction of impurities/ biomolecules.

Quantum transport method provides detailed and accurate information about the transport properties in the nanoscale. Therefore, the interaction of biomolecule with the proposed 2D materials used for sensing will be investigated by using DFT and non-equilibrium Green's function approach implemented in SIESTA/Transiesta and/or commercial tools like Quantumwise ATK.

Proposal 2 : Investigations on electrodes and performance analysis of polymeric electrochemical and Photovoltaic devices

To meet the ever-increasing energy demands and sustainability requirements, next-generation battery systems must provide superior energy densities while employing eco-friendly components. Exploiting materials from biological systems, or bio-inspiration, offers an alternative strategy to overcome the conventional energy storage mechanism through the chemical diversity, highly efficient biochemistry, sustainability, and natural abundance provided by these materials. Proposed work is categorized as :

Designing, structural and stability analysis of new electrodes and active materials.
Mechanical strength analysis of polymeric systems.
Electronic and optical properties study with different physical conditions.
Designing of electrochemical and/or photovoltaic device and their I-V characteristics analysis and computation of important parameters.

Performance analysis of devices.

Work will be extended upto the modeling of bio-batteries, bio-capacitors and bio-solar cells.

The fabrication of devices (with best performance) may be the next part of this proposal(I have experimental experience of fabrication of solid state batteries and supercapacitors).

SIESTA /Ttransiesta and/or commercial tools like Quantumwise ATK will be used for the different computational analysis. I am searching for a good tool for modeling of solar cell i.e. to study the photon-electron interaction.

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