

## **University School of Basic & Applied Sciences Guru Gobind Singh Indraprastha University**



### Organizes Workshop

on

# Atomistic modelling using Synopsys QuantumATK for Nanomaterials/ Nano Devices

### **PATRON**

### Hon'ble Vice Chancellor Padma Shri Prof. (Dr.) Mahesh Verma

#### TOPICS TO BE COVERED

- INTRODUCTION TO QUANTUMATK SOFTWARE
- TYPES OF SIMULATORS IN QUANTUMATK
- GENERAL WORK-FLOW IN QUANTUM ATK
- (DFT) DENISTY FUNCTIONAL THEORY
- (NEGF) NON-EQUILIBRIUM GREEN FUNCTION
- ADVANCED CALCULATION AND ANALYSIS
- MATERIAL BUILDING LIBRARY
- OPTIMIZATION OF GEOMETRY
- SCIPRTING IN QUANTUMATK
- LIVE DEMONSTRATION OF QUANTUM ATK
- VIRTUAL NANO LAB (VNL)
- NANO-STRUCTURED MATERIALS AND DEVICES
- ATOMISTIC MODELLING
- BULK/ MOLECULE CONFUGURATION
- DOPING AND SPATIAL REGION FOR DEVICES

27<sup>th</sup> October, 2023 (11:00 am - 4:00 pm) Please Register at URL:

https://forms.gle/fRX7AVqP6QdYb9Ze9

Convener: Dr. Anjana Bagga

Contact: Dean

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