

## Seminar/Talk

## Multi-Scaled Simulations and Modelling of Novel Materials and Electronic Devices

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Host: Georgios Katsaros

Recently, interest in electronic, magnetic and optical materials based on inorganic and organic nanomaterials has increased significantly. Such new materials and novel device architectures have the potential to bring the technology beyond the Moore era. The most time-efficient and cost-effective approach to finding the best materials and devices for specific applications is to perform modelling and simulations. In this talk, I will present exciting research carried out by my research group, DeepNano, in the fields of biosensors, molecular electronics, superconducting qubits and the variability of nano-scale transistors to show the importance of material modelling and device simulations not only in academia but also in the industry. Our main aim is to establish a link between the material properties, device architecture and performance using hierarchical, multi-scaled simulation modelling. For example, to evaluate the performance of superconducting qubits, we have developed a simulation flow that links the atomistic simulations with a three-dimensional (3D) numerical device simulator. Also, to simulate the electrical and optical response of biosensors, we have combined analytical and machine learning (ML) methods in a unified simulation framework. In this way, the computation flows and numerical methods developed in my research group can evaluate the material properties and device performance of various heterogeneous devices and systems.

## Wednesday, April 17, 2024 09:30am - 10:30am

Mondi Seminar Room 2, Central Building



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