Evento organizzato nell'ambito di Engineering Physics Colloquia

Numerical Simulation of Transport in Large-Area Disordered Materials

Ca' Foscari University of Venice
Department of Molecular Sciences and Nanosystems

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Conference Room Orio Zanetto, Alfa Building - Scientific Campus, Via Torino 155, Mestre (Venezia)

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Gli organizzatori offriranno coffee & cookies ai partecipanti

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Organizzazione di
Domenico De Fazio

In nano- and mesoscale systems, defects and disorder play a fundamental role in determining material properties and device performance. Such defects and disorder often present themselves on the atomic or sub-nanometer scale, while resulting transport length scales or device sizes can be orders of magnitude larger, on the micron scale. To accurately quantify and predict material properties or device performance in such situations, one often needs modeling and simulation tools that can bridge the size gap between atomic-scale defects and micron-scale systems.
In this talk, I will present our group's linear-scaling quantum transport tool, called LSQUANT. Based on the Kubo transport formalism, this tool combines accurate tight-binding models with an efficient expansion of quantum operators to allow the simulation of transport in systems containing many millions of atoms. This enables an atomic description of defects and disorder while still resolving transport properties on the experimental scale.
After an introduction to the LSQUANT methodology, I will present a few examples of its application to transport in graphene, including spin and charge transport in disordered single-layer graphene and graphene nanoribbons. Time permitting, I will also discuss recent efforts to update the LSQUANT methodology to study energy absorption and emission and the time-resolved dynamics of systems driven out of equilibrium, with an eye toward applications in photodetection, sensing, and optical communications.