

How electrons move in organic materials

Electricity and electronics are examples of technologies that are based on transport of charge (electrons) through materials. Understanding and development of electron transport properties of materials is therefore of fundamental interest and importance for the development of modern society.

In this presentation I will review the theoretical models that are used to describe charge transport in carbon based materials, including Nobel Prize awarded novel materials such as fullerenes (NP chemistry 1996), conducting polymers (NP chemistry 2000). Also organic “materials” such as molecules for photosynthesis and DNA will be discussed in this context. It is evident from this list of materials that carbon can exist in different chemical bonding states. This is one of the clues to explain how carbon based materials can range from highly conducting to nearly insulating. The ability to control and explore the rich carbon chemistry is one of the most challenging problems in materials science today.

At the end of my talk I will also present the National Supercomputer Centre at LiU and some of the applications for which high performance computing and data storage is an absolute necessity.