数学与系统科学研究院

计算数学所学术报告

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报告题目：

From micro to molecular electronics: a first-principles approach

邀请人：　　周爱辉研究员

报告时间：**2011** 年 **11** 月 **18** 日（周五）

上午 **10：00-11：00**

报告地点：　　科技综合楼三层 **311**

计算数学所报告厅

Abstract:

From the cellular phone to the personal digital assistant, miniaturization is omnipresent in our everyday life. Typical electronic components are now reaching dimensions smaller than 10 nm: we have entered the nanoelectronics era. Understanding the interfaces of materials of very different nature has become more and more a critical issue. Indeed, the components are based on the coupling of semiconductors, metals, superconductors, magnetic materials, dielectrics, organic molecules, or biological systems.

In this respect, nanoelectronics can greatly benefit from computer simulation techniques and more particularly from first-principles calculations. In this lecture, I will present a few recent results about materials for electronics obtained using DFT and MBPT. On the one hand, I will discuss the band offsets and the defect levels at various interfaces. On the other hand, I will show some quantum transport calculations on molecular devices.

欢迎大家参加！