数学与系统科学研究院

计算数学所短期课程

报告人：Prof. Gian-Marco Rignanese

（ Catholic University of Louvain ）

报告题目：

Electronic band structures of solids from first-principles

邀请人：　　周爱辉 研究员

报告时间：

I. 2015 年 6 月 1 日（周一）下午 15:00-17:00

II. 2015 年 6 月 3 日（周三）上午 9:00-11:00

III. 2015 年 6 月 10 日（周三）上午 9:00-11:00

报告地点：　　科技综合楼三层

311 报告厅

Abstract:

Starting from the basics of solid state physics (including crystallography and diffraction), this lecture will present various methods for calculating electronic band structures from first-principles. Today, Density Functional Theory (DFT) is one of the most widely used methods for ground-state properties. In contrast, excited-states properties are not properly described by DFT. For this reason, in the last years, efficient and reliable first-principles theories and frameworks have been devised to describe electronic excitations. These new tools are becoming more and more used: time-dependent density-functional theory (TDDFT) and the Many-Body Perturbation Theory (MBPT) in the GW approximation and Bethe-Salpeter equation (BSE). The aim of this lecture is to introduce the concepts underlying those different methods and to apply them on real systems. Theoretical sessions will be followed by extensive hands-on classes. Participants will have the opportunity of testing the theoretical methods using the ABINIT code on dedicated tutorials.

欢迎大家参加！