# 数学与系统科学研究院

# 计算数学所学术报告

**(系列报告)**

**报告人： Prof. Reinhold Schneider**

**(Teschnische Universitaet Berlin, Germany)**

**报告题目：**

**The Comptuation of the Electrnic Structure –Numerical Methods in Quantum Chemistry**

**邀请人： 周爱辉研究员**

**报告时间：**

1. **2009 年 8 月 5 日(周三)**

   **下午 2:30—5:20**

2. **2009 年 8 月 12 日(周三)**

下午 2:30—5:20

3. 2009 年 8 月 19 日(周三)

下午 2:30—5:20

4. 2009 年 8 月 26 日(周三)

下午 2:30—5:20

**报告地点：** 科技综合楼三层 311

计算数学所报告厅


## Abstract:

**The stationary electronic Schr\''odinger provides quantum mechanical model for an $N$−electron system inside the electro−static field given by fixed nuclei. One is mainly interested in the lowest eigenvalues. Since the eigenfunctions depends on 3N spatial and N spin variables $s_i =\pm\{\frac{1}{2} \}$, even for small molecules, this is an eigenvalue problem in high dimensions. Hartree Fock and Density Functional Theory reduce this problem ot a**

**highly nonlinear problem in 3 dimensions and provide affirmative answers also for relatively large systems. To achieve better accuracy, requires a size consistent approximation of wave function. In case of dynamical correlation, the CC (coupled cluster) method provides the most accurate results. Open shell systems, with a high amount of statical correlation cannot be treated by such single reference methods. Density matrix minimization and Density Matrix Functional Theory offer some new perspectives for this challenging and hard problems.**

欢迎大家参加！