

数学与系统科学研究院

计算数学所学术报告

报告人: **Prof. Chao Yang**

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报告题目:

**Sparse Correction in Coupled
Cluster Calculations**

邀请人: 周爱辉 研究员

报告时间: **2015 年 11 月 20 日 (周五)**

上午 10: 00-11: 00

报告地点: 数学院南楼九层

902 会议室

Abstract:

The coupled-cluster method is a highly accurate wavefunction method solving a many-body Schrodinger's equation. However, its computational complexity scales as $O(N^6)$, where N is the number of electrons. In this talk, we discuss a technique for reducing the cost of coupled-cluster calculation by exploiting the sparsity of the correction tensor in an inexact Newton method for solving the coupled-cluster nonlinear equation.

欢迎大家参加！