# 数学与系统科学研究院

# 计算数学所学术报告

**报告人：　Dr. Yuzhi Zhou**

*（ Department of Materials Science and Engineering,*

*University of California at Berkeley ）*

**报告题目：**

**Theoretical investigations of functional material: TlBr**

**邀请人：　　戴小英 副研究员**

**报告时间：2016 年 7 月 20 日（周三）**

**下午 16:00-17:00**

**报告地点：　　数学院南楼六层**

**602 会议室**

## Abstract:

**I will present the theoretical investigations of anovel functional material: TlBr.**

**TlBr is interesting due to its potential application as a high-quality room temperature radiation detector. The stability and electronic structures of three phases of TlBr are studied using Density Functional Theorem (DFT) calculations employing a hybrid functional (PBE0). The calculated band gaps from DFT with the hybrid functional are in excellent agreement with experimental measurements. The influence of some interstitial and substitutional dopants on TlBr properties is further studied. DFT predicts that interstitial and substitutional C, N, and O dopants in TlBr can display large, localized magnetic moments. A simple model that employs Pauli exclusion principle and group theory is introduced to explain the origin and magnitude of the moments.**


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