数学与系统科学研究院

计算数学所学术报告

报告人： **Dr. Daniel Massatt**

（ ***University of Chicago*** ）

报告题目：

Electronic Structure of Relaxed Incommensurate 2D Heterostructures

邀请人： 周爱辉 研究员

报告时间：**2019** 年 **9** 月 **17** 日（周二）

上午 **10:00-11:00**

报告地点： 数学院南楼二层

212 教室

Abstract:

2D materials have extensive potential application in optics and electronics due to their unique mechanical and electric properties. How to numerically simulate electronic properties is well understood for periodic atomistic lattices, but has been unknown for materials that are stacked with misalignment that breaks the periodicity of the ensemble, i.e., incommensurate materials. The previous approach has been to artificially strain the layers to be able to use the theory and computational methods for periodic systems.

We show how to rigorously define the electronic density of states (DOS) for two-dimensional incommensurate layered structures, where Fourier-Bloch theory does not apply, and efficiently approximate it using a novel configuration space representation and locality technique. We have also been able to apply our configuration space approach to obtain mechanical relaxation patterns using a continuum elasticity model coupled with a stacking energy model. We combine these two models together to form an electronic structure calculation for an incommensurate system with atomistic relaxation.

欢迎大家参加！