THE UNIVERSITY OF CHICAGO

COMPUTATIONAL AND APPLIED MATHEMATICS COLLOQUIUM

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Twists and Misfits: Mathematical Modeling for Incommensurate 2D Materials

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Jones 226, 5747 South Ellis Avenue

ABSTRACT

Two-dimensional crystals have been intensely investigated both experimentally and theoretically since graphene was exfoliated from graphite. Physicists have recently developed the ability to stack one layer on another with a twist angle controlled to the scale of .1 degree with the goal of creating two dimensional materials with desired electronic, optical, and mechanical properties.
Unusual geometries appear at the atomic-scale, such as lattice mismatches, twist angles and Moire patterns, providing new challenges for our fundamental understanding.
One of the main issues encountered in the mathematical and computational modeling of 2D materials is that misalignments between the layers destroy the periodic character of the system.

We discuss novel mathematical models for the analysis and computational prediction of mechanical relaxation of two-dimensional layered atomic crystals in the presence of large-scale moiré patterns.
The concept of configuration space or hull, previously introduced for the study of transport properties in aperiodic materials by Belissard et al., is shown to allow for a unified description of mechanical as well as electronic structure models for any materials in the truly incommensurate (aperiodic) regime.

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