



THE UNIVERSITY OF CHICAGO

COMPUTATIONAL AND APPLIED MATHEMATICS COLLOQUIUM

MITCHELL LUSKIN

School of Mathematics
University of Minnesota

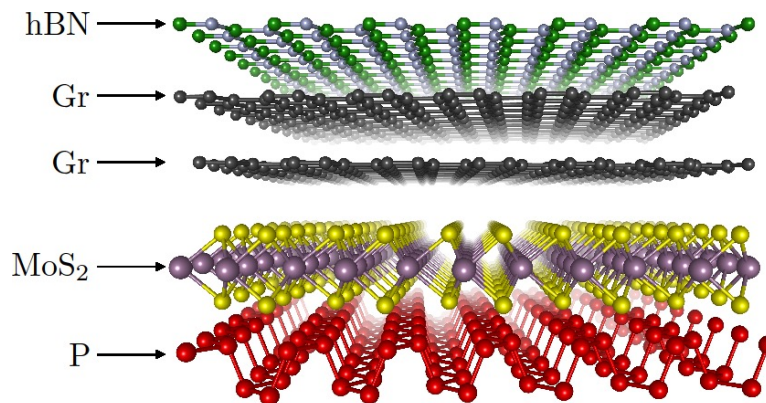
ABST Mathematical Modeling and Numerical Analysis for Incommensurate 2D Materials

THURSDAY, April 25, 2019, at 4:00 PM
Jones 226, 5747 South Ellis Avenue

ABSTRACT

One atom thick, two dimensional crystalline layers of atoms have recently been extracted. Stacking a few layers of these 2D materials such as graphene and molybdenum disulfide at controlled twist angle has opened the possibility of tuning the electronic and optical properties of 2D materials. One of the main issues encountered in the mathematical and computational modeling of 2D materials is that lattice mismatch and rotations between the layers destroys the periodic character of the system.

Basic concepts like the elastic relaxation and electronic density of states (eigenvalue distribution of the Hamiltonian) will be formulated and analyzed in the incommensurate (aperiodic) setting. We have developed a novel variational model for the elastic relaxation and new methods to compute the distribution of eigenvalues for the incommensurate Hamiltonian. New computational approaches will be presented, and the validity and efficiency of these approximations will be examined from mathematical and numerical analysis perspectives.



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Organizers:

Daniel Sanz-Alonso, Department of Statistics, sanzalonso@uchicago.edu
CAM Colloquium URL: <https://cam.uchicago.edu/seminars/colloq/index.shtml>.

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