# The Hong Kong University of Science and Technology

## Department of Mathematics

## <u>Seminar on Applied Mathematics</u>

### Dislocation network structures in bilayer sheet
### *by*

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**Wuhan University**

#### <u>Abstract</u>

We develop a multiscale continuum model to describe the interlayer defects in bilayer materials. The model incorporates both the anisotropy elasticity of each mono-layer in bilayer materials and the first-principle calculation informed interaction between two layers, i.e., the nonlinear atomistic potential energy between two layers. The equilibrium structures are obtained from the numerical simulations of the force balance differential equations. We apply this approach to determine the structure and energetics of twisted bilayer material. In tBLG, two distinct, modified Moiré structures are observed. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.

*Date:*        *Friday, 18 Aug 2017*

*Time:*        *4:00p.m. – 5:00p.m.*

*Venue:*       *Room 4504, Academic Building*
*(near Lifts 25 & 26), HKUST*

### *All are welcome!*