

**October 25**, 2021 10:00 AM  
QED & Materials seminar  
**Yang Zhang (MIT Physics)**

**Title**

**" Quantum Chemistry, correlation and topology in semiconductor moiré"**

**Abstract**

Transition metal dichalcogenide (TMD) based moiré materials have been shown to host various correlated electronic phenomena including Mott insulating states and fractional filling charge orders, quantum anomalous Hall and quantum spin Hall effect. To describe the low energy electronic states of long wavelength moiré superlattice, we introduced the concept of moiré quantum chemistry and developed the density functional theory to study the filling dependent insulating state and emergent magnetic properties [1,2]. In twisted homobilayer MoS<sub>2</sub>, we proposed the electrical tunable charge order and interaction induced Mott ferroelectricity [3].

More recently, we developed the theory of topological moiré bands in AB-stacked TMD heterobilayers [4,5]. Valley contrasting Chern bands with non-trivial spin texture are formed from interlayer hybridization between moiré bands of nominally opposite spins. This work establishes a recipe for creating topological states in AB stacked TMD bilayers by tuning the displacement field, which provides a highly tunable platform for realizing quantum spin Hall and interaction induced quantum anomalous Hall effects. These series of work reveal rich physics of semiconductor moiré superlattices as manifested in a variety of correlated and topological states.

[1] Y Zhang, N Yuan, L Fu, PRB 102 (20), 201115

[2] Y Zhang, H Isobe, L Fu, arXiv:2005.04238

[3] Y Zhang, T Liu, L Fu, PRB 103 (15), 155142

[4] Y Zhang, T Devakul, L Fu, PNAS 118 (36), 2021

[5] T Li, et al, arXiv:2107.01796