“Catalysis and topology in moiré semiconductor and metal.”

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 (spin) Hall effect. We introduced the concept of moiré quantum chemistry to study the filling dependent insulating state and emergent magnetic properties [1]. Moreover, the richness of local chemical environment in moiré structures provides an advantageous and versatile method to increase chemical reaction speed [2]. As a hydrogen evolution reaction catalyst, twisted NbS₂ is shown to cover the thermoneutral volcano peak, exceeding the efficiency of the current record platinum.

More recently, we developed the theory of topological moiré bands in AB-stacked TMD heterobilayers [3,4]. These series of work reveal rich physics of moiré superlattices as manifested in a variety of correlated and topological states, and the application for chemical reaction.

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