ABSTRACT

My thesis work consists of two verticals - one on quantum materials applications of p-block mono-layers and the other on methodological developments. In the first vertical I started with contributing to our group effort in developing optimally directed hybrid atomic Wannier orbital basis and subsequently developed a real space formalism to partition the total charge density into densities of charges retained by atoms and shared between them. In the second vertical, I started with exploring the evolution of electronic structure of lighter p-block monolayers - Xenes, and found the possibility of in-plane electromechanical actuation in covalent monolayers.

On the first vertical consisting of methodological development, I will first briefly demonstrate construction of optimally directed hybrid atomic Wannier orbital basis in covalent systems with non-ideal bond angles, guided by the Mayer's bond order and subsequently discuss our derivation of spatial distribution of bond order rendering division of total charge in the system into densities of charges shared among atoms and retained by them, in a representative set of systems.

On the second vertical containing application to materials, I will begin with Xanes and demonstrate the general feasibility of reversibly tuning the properties of monolayers constituted by three coordinated lighter p block atoms through the application of inhomogeneous bias using experimentally realisable gate configurations. I will demonstrate from first-principles the reversible emergence of a topological insulator (TI) phase in germanane and stanane via in-plane, electrically induced strain. By applying non-uniform gate bias at realistic length scales, robust uniaxial strain is generated, driving a transition from trivial insulator to weak and then strong TI phases. This electro-mechanical tuning, also observed in nano-ribbons and supported by Kane-Mele model analysis, offers a promising route to controllable topological states in 2D p-block covalent networks. Employing a similar electric field profile in graphene/hBN in-plane heterostructures results in strain-assisted half-metallic behavior, highlighting the tunability of electronic properties through electro-mechanical actuation in lateral 2D systems. Subsequently, I move on to graphene and show that by application of an inhomogeneous bias, resultant inhomogeneous in-plane electric field modulates the band structure of graphene via the induced inhomogeneous strain.