

**NUS Graduate School for Integrative Sciences and Engineering  
Research Project Write-up**

**Title of Project :**           Advanced 2D materials (graphene and beyond graphene) and their device applications

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**Short Description**

Investigating material properties is the most essential step in any study on devices. Therefore, advanced models, such as *ab-initio* calculations, semi-empirical tight-binding and pseudo-potential methodologies, are implemented in the different levels to appropriately understand the electronic structures and phonon dispersion relations of novel nanostructures including graphene-based and beyond graphene materials. Furthermore, strain/stress effects and scattering processes are also investigated based on different mechanisms such as impurity, surface (edge) roughness, and phonon-electronic interactions. The materials we focused on are widely included carbon-based materials such as graphene, monolayer and bilayer graphene nanoribbon, and beyond graphene systems  $(\text{BN})_x\text{C}_y$  hybridized systems,  $\text{MoS}_2$ , Silicene, etc. Our works explored the rich electronic and magnetic behaviors in these systems, and we have established the mechanism to clarify the physics behind these observations. After exploiting these unique and promising features, novel functional devices can be further studied. We aim to explore their potential device applications in nanoscale FETs, quantum tunneling FETs, and spintronic devices.