

## **Webinar**

**The effect of deformation, twist and strain in the van der Waals layered systems: An ab initio study**

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The Monte Carlo Simulations reveal the possibility of stable new deformation called ripplocation and also the formation of ripple in Graphene with the compressive strain. Unlike the conventional dislocations, the ripplocation is a non-trivial, multivalued, out of plane fluctuations. First, I will discuss the electronic, magnetic and optical properties of ripplocation and ripple in graphene using first principles calculations based on Density functional theory. In the second part, I will briefly discuss the work related to the origin of direct band gap noticed in MoS<sub>2</sub> multiplayers grown on SrTiO<sub>3</sub>. In the final part, I will show an analytical study of Debye temperature that fits the experimental data of volume variation of WSe<sub>2</sub> with temperature especially in the range from 111K to 400K.

***Monday, Feb 22<sup>nd</sup> 2021***

***11:30 AM***