**Modeling the Flatland from Atoms and Up**

Yuanyue Liu

Division of Applied Physics and Materials Science, Division of Chemistry and Chemical Engineering, Materials and Process Simulation Center, and The Resnick Sustainability Institute

California Institute of Technology, Pasadena, CA, 91125

yuanyue@caltech.edu

Advances in materials have continuously revolutionized our life. Two-dimensional (2D, i.e. atomically thin) materials have attracted great interest in recent years due to their intriguing fundamental properties and promising applications. Yet their full potential is still limited by a number of challenges. I will discuss some examples in which we use theory and computational methods to help solve some of the critical problems, such as: how to grow a high-quality and large-scale crystal1-7, how to passivate/engineer the defects8-14, and how to reduce the contact resistance for charge carrier transport15, 16. These progresses are made by uncovering the relations between atomic structures and properties. I will also show how the underlying electronic factors control the binding strength of adsorbates with 2D materials, the understanding of which leads to improvement of material performance and discovery of new materials for energy storage (batteries17-19) and conversion (water to fuels20, 21). These studies could help advance electronics and clean energy towards next-generation, and also serve as a basis for development of interdisciplinary computational materials design projects, such as materials interface/defects genome.

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