



### Seminar

## Raman Spectroscopy of Interlayer Phonons in Transition Metal Dichalcogenide Atomic Layers

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**Time: 10:00am, June 23, 2017 (Friday)**

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**Venue: Room W563, Physics building, Peking University**

**地点: 北京大学物理楼, 西663会议室**

### Abstract

Atomically thin  $\text{ReS}_2$  and  $\text{NbSe}_2$  crystals are new types of 2D materials that have different crystal structures and electronic properties from common transition metal dichalcogenides (TMDs), e.g.  $\text{MoS}_2$ ,  $\text{MoSe}_2$ ,  $\text{WS}_2$ , and  $\text{WSe}_2$ . We measured ultralow frequency Raman response of  $\text{ReS}_2$  and  $\text{NbSe}_2$  atomic layers.  $\text{ReS}_2$  has unique distorted 1T structure. We found that the two shear phonon modes in bilayer  $\text{ReS}_2$  are nondegenerate and clearly resolved in the Raman spectrum, in contrast to the doubly degenerate shear modes in other TMD materials. By carrying out comprehensive first-principles calculations, we can account for the frequency and Raman intensity of interlayer modes and determine the stacking order of bilayer  $\text{ReS}_2$ . Few-layer  $\text{ReS}_2$  exhibits rich Raman peaks at frequencies below  $50 \text{ cm}^{-1}$ , where a panoply of interlayer shear and breathing modes are observed. Atomically thin  $\text{NbSe}_2$  is a metallic layered TMD with novel charge-density-wave (CDW) and superconductive phases. We observed both the interlayer breathing modes and shear modes at frequencies below  $40 \text{ cm}^{-1}$  for samples of 2 to 15 layers. Their frequencies, Raman activities, and environmental instability depend systematically on the layer number. We find that, although  $\text{NbSe}_2$  has different stacking order from  $\text{MoS}_2$ , they share the same crystal symmetry groups and exhibit similar Raman selection rules for interlayer phonons. In addition, the interlayer phonon modes evolve smoothly from  $T = 300 \text{ K}$  to  $8 \text{ K}$ , with no observable response to the CDW formation in  $\text{NbSe}_2$ . Our results reveal that the interlayer phonons can serve as an effective probe of the interface properties and interlayer interactions in these 2D atomic layers. In the third part of my talk, I will present our recent studies of nearly commensurate to commensurate CDW transitions in ultrathin 1T-TaS<sub>2</sub>. We identified additional CDW modes from surface layers of 1T-TaS<sub>2</sub>. Phase nucleation energetics are proposed to understand the bulk and surface CDW transitions.

### About the speaker

Dr. He, Rui obtained her B.S. degree from Fudan University in China in 1999. She received her Ph.D. degree in Applied Physics from Columbia University in the US in 2006. After her graduation from Columbia, she joined the Hong Kong University of Science and Technology as a postdoc in the physics department and as a research assistant in the mathematics department. In 2009 she returned to Columbia University where she worked as a postdoctoral research scientist. She joined the Physics Department at the University of Northern Iowa in August 2011. She will move to Texas Tech University in July 2017. Her research interests include the general area of optical studies of nanostructures including atomic layers of graphene, low-dimensional dichalcogenide crystals, and heterostructures formed from these 2D crystals.