GRADUATE STUDENT RESEARCH SEMINAR SERIES (2017)

STRAIN AND DEFECT ENGINEERING ON NEW GENERATION NANO-SEMICONDUCTOR SINGLE LAYER MOS 2

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Single layer MoS 2 is a promising candidate in the application of NEMS (nanoelectromechanical systems) due to its minimal size and excellent electro-mechanical properties. Unlike earlier discovered two-dimensional semiconductor materials, such as graphene with a vanishing band gap, single layer MoS 2 has a band gap of 1.8 eV which is within the visible light range. It indicates that single layer MoS 2 is ideal for the application of nano-optical devices. Single layer MoS 2 can experience various loading conditions during actual operation, such as strain and defects. Moreover, these two types of perturbation are often effective methods to engineer semiconductor properties. Therefore, in this work, we focused on the evolution of mechanical and electrical properties of single layer MoS 2 with strain and defects. With DFT calculation, it is revealed that both strain and defects have great impact on the performance of single layer MoS 2 . Uniaxial tensile tests show that single layer MoS 2 responds to applied strain differently with change in strain orientation. Defects such vacancies can decrease the strength and stiffness of single layer MoS 2. In addition, with increasing uniaxial tensile strain, the band gap decreases to about 0.5 eV upon failure. Such variation leads to red shift of the light emitted by single layer MoS 2. The introduction of defects can create intermediate states in the band structures therefore affecting the band gap energy. These results demonstrate that both strain and defects are effective in tuning the properties of single layer MoS 2 and can be utilized to extend its application.

MONDAY, SEPTEMBER 18 AT 3:00-4:00 PM

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