



Department of  
Mechanical Engineering  
The University of Hong Kong



## SEMINAR

# **A DFT Study of Novel Out-of-plane Second Harmonic Generation and Its Enhancement in Monolayer Transition Metal Dichalcogenides**

**Date:** 20 April, 2023 (Thursday)

**Time:** 11:00 a.m.

**Venue:** Room 7-34, Haking Wong Building, HKU

**Speaker:** Mr. Guan Zhizi (PhD candidate)  
Department of Mechanical Engineering  
The University of Hong Kong

### **Abstract:**

Two-dimensional (2D) materials have attracted tremendous attention in nonlinear optics due to their unique electronic and optical properties. Among these materials, transition metal dichalcogenides (TMDCs) monolayers with broken in-plane crystal inversion symmetry have shown great promise in second harmonic generation (SHG) because of their large nonlinear susceptibility. However, inducing and detecting their out-of-plane polarized SHG are challenging, limiting the potential application in nonlinear optics. This study investigates the possibility of inducing novel out-of-plane SHG in TMDCs monolayers. Our calculations show that the out-of-plane SHG susceptibility induced by the electric field can be comparable to the intrinsic in-plane component around the visible light range. Furthermore, we propose a new band nesting mechanism that can enhance the out-of-plane SHG susceptibility by 4 to 5 times. Our work provides a potential approach for future experiments and offers unique opportunities for exploring and designing nonlinear optical properties in 2D materials.

**ALL INTERESTED ARE WELCOME**

For further information, please contact Prof. D.J. Srolovitz at 3917 2800.