



## Weekly Seminar

# Insights into exotic quantum materials via first-principles hyperfine coupling calculations

**Zheng Liu**

*Tsinghua University*



**Time: 3:00 pm, Dec. 20, 2023 (Wednesday)**

**时间: 2023年12月20日 (周三) 下午3:00**

**Venue: Room w563, Physics building, Peking University**

**地点: 北京大学物理楼, 西563会议室**

### Abstract

In a condensed matter system, the hyperfine levels of nuclei reveal important information on the electronic properties, based on which novel experimental techniques are developed. In the computational physics community, meanwhile, decades of efforts have also been made to reliably predict the key ingredients governing the hyperfine splitting in first principle, such as the hyperfine coupling constant and the electric field gradient at a nuclear site. This talk aims to show that by carefully designing the calculation, this computational power can be extended to exotic quantum materials, which further provides useful clues to understand novel experimental observations. The discussion will mainly be based on frustrated or seemingly frustrated magnets, including  $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$ ,  $\text{Cu}_3\text{Zn}(\text{OH})_6\text{FBr}$ ,  $\text{CaFeTi}_2\text{O}_6$  and  $1\text{T-TaS}_2$ .

### About the speaker

Zheng Liu is currently a member at Institute for Advanced Study, Tsinghua University. He works on the intersection of condensed matter physics and materials science, particularly focusing on bridging the theoretical frontier with first-principles calculation.