北京大学量子材料科学中心
International Center for Quantum Materials, PKU

Seminar

First-Principles Materials Theory, Discovery and Design of Electronic and Optoelectronic Materials

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Venue: Room W563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

Recent advances in first-principles electronic structure theory and high-performance high-throughput computing have empowered efficient computation-aided discovery and design of novel materials, particularly important for emerging energy and device technologies. In this talk, I will highlight a few examples of our work on materials discovery and device design enabled by first-principles theory. First, I will present theoretical discovery and experimental investigations of 2D and 3D topological materials including Peierls-distorted 1T' and T_d binary and ternary transition metal dichalcogenides (WTe_2, $MoTe_2$, $TaIrTe_4$, $TaRhTe_4$, $NbIrTe_4$, $NbRhTe_4$). We will also discuss the electric field, elastic strain, and van der Waals stacking induced topological phase transition and their potential applications for topotronics such as topological field effect transistor. Second, I will report our recent discovery of strongly coupled ferroelectric-ferroelastic multiferroics in 2D group IV monochalcogenides. These 2D multiferroics possess a few distinct characteristics including strongly-coupled giant ferroelectricity and ferroelasticity, large anisotropic excitonic optical properties with visible-spectrum excitonic gaps and sizable exciton binding energies, and low domain wall energy and migration barrier, suggesting their great potentials for tunable multiferroic functional devices by manipulating external electrical, mechanical, and optical field to control the internal physical responses, such as 2D multiferroic memories, ferroelectric excitonic photovoltaics, and nonvolatile multiferroic photonic memory. Finally, I will present some first-principles methodology development towards more accurate and efficient predictions to expedite high-throughput materials discovery and design for novel energy and device applications..

About the speaker

Dr. Xiaofeng Qian is an assistant professor in the Department of Materials Science and Engineering at Texas A&M University, working on first-principles materials theory, discovery, and design for energy and device applications. Dr. Qian obtained his bachelor's degree in Engineering Physics from Tsinghua University in China in 2001, and received his Ph.D. degree in Nuclear Science and Engineering from Massachusetts Institute of Technology in 2008. He then worked with Prof. Nicola Marzari and Prof. Ju Li as a postdoc at MIT on the first-principles excited state methodology and 2D materials and device design, and joined Texas A&M University in 2015. His group is currently focusing on first-principles theory of light-matter interaction at the nanoscale.