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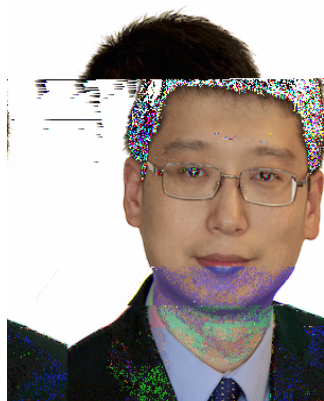
International Center for Quantum Material PKU

Seminar

First-Principle Material Theory, Discovery and Design of Electronic and Optoelectronic Material

Xiao Qian

Department of Material Science and Engineering
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Time: 4:00, Aug. 11, 2017 (Friday)

时间: 2017年8月11日 (周五) 下午4:00

Venue: Room W563, Physics Building, PKU

地点: 北京大学物理楼, 西563会议室

Recent advance in first-principle electronic structure theory and high-performance high-throughput computing have empowered efficient computer-aided discovery and design of novel material, particularly important for emerging energy and device technologies. In this talk, I will highlight a few examples of our work on material discovery and device design enabled by first-principle theory. First, I will present theoretical discovery and experimental investigation of 2D and 3D topological material including Peierl-dimerized 1T and 2D binary and ternary transition metal dichalcogenide (WTe_2 , MoTe_2 , TaI-Te_4 , TaRhTe_4 , NbI-Te_4 , NbRhTe_4). We will also discuss the electric field, elastic strain, and Landé-Waals stacking induced topological phase transition and their potential application for optoelectronic chiral topological field effect transistor. Second, I will report our recent discovery of strongly coupled ferroelectric-ferroelastic multiferroic in 2D group IV monochalcogenide. The 2D multiferroic possesses a few distinctive characteristics including strongly coupled giant ferroelectricity and ferroelasticity, large anisotropic dielectric optical properties with tunable piezoelectric gap and tunable dielectric binding energy, and low domain wall energy and migration barrier, giving high potential for tunable multiferroic functional device by manipulating external electrical, mechanical, and optical field to control the internal physical response, such as 2D multiferroic memory, ferroelectric dielectric photovoltaic, and nonvolatile multiferroic photonic memory. Finally, I will present some first-principle methodology development and more accurate and efficient prediction to predict high-throughput material discovery and design for novel energy and device application...

Dr. Xiaofeng Qian is an assistant professor in the Department of Material Science and Engineering at Texas A&M University, working on first-principle material theory, discovery, and design for energy and device application. 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. J. Li as a postdoc at MIT on the first-principle electronic structure methodology and 2D material and device design, and joined Texas A&M University in 2015. His group's current focus is on first-principle theory of light-matter interaction at the nanoscale.