# 北京大学量子材料科学中心

International Center for Quantum Materials, PKU

## Weekly Seminar

# Complex wave vector band structure for quantum transport


**Xiaoguang Zhang**

*University of Florida*


**Time: 4:00pm, May 18, 2016(Wednesday)**

**时间：2016年5月18日 （周三）下午4:00**

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

**地点：北京大学物理楼，西563会议室**

## Abstract


Quantum mechanically forbidden states in a solid can exist as exponentially decaying states at surfaces and interfaces. These decaying states are described by complex wave vectors whose imaginary parts determine their rates of decay. The energy dependence of these complex wave vectors for a solid, the so-called complex band structure, can help us determine quantum transport properties of the material entirely from first-principles (i.e., without adjustable parameters that are fit to experiments). Complex band structure calculation was instrumental in the successful prediction of giant tunneling magnetoresistance in magnetic tunnel junctions. Here we show how complex band calculations can be extended 1. to predict negative differential resistance in magnetic tunnel junctions with narrow gap barrier layers, specifically those using so-called cubic cation disordered crystals (CCDC's); 2. to estimate resistance of twin grain boundaries in copper; and 3. to calculate electron mobility in silicon due to impurity and phonon scattering. Comparison with experiments in cases 2 and 3 shows that complex band structure provides a powerful and accurate method for quantum transport.


## About the speaker

Xiaoguang Zhang received his BS degree in Physics from Peking University in 1983, and got Ph.D. degree in Physics from Northwestern University in 1989. His research interests focus on theory and modeling of electron transport in magnetic tunnel junctions, molecular junctions, polymers and nanoscale materials; calculation of electron mobility and defect capture cross section in semiconductors; image informatics for scanning tunneling potentiometry.