

## 凝聚态物理前沿论坛

## 第七十九讲

题 目: Theoretical Study of Defect Properties

in Semiconductors

报告人: 魏苏淮教授北京计算科学研究中心

时间: 2019年11月6日(周三) 下午2:00~5:00

地 点: 固体所新楼520会议室

报告摘要: In this talk, I will first discuss some general concepts of defects in semiconductors and discuss in detail the first-principles defect calculation methods based on supercell approach; then I will discuss the origin of the doping difficulties in semiconductor materials and the approaches one may use to overcome the doping bottleneck in these materials, including (1) how to increase defect solubility by "defeating" defect thermodynamics using non-equilibrium approaches; (2) how to reduce defect ionization energy level by designing shallower dopants or dopant complexes; and (3) how to reduce defect compensation and ionization level by modifying the host band structure near the band edges.

报告人简介: Professor Su-Huai Wei is a Professor at the Beijing Computational Science Research Center (CSRC). He received his B.S. in Physics from Fudan University in 1981 and Ph.D. from the College of William and Mary in 1985. He was a Laboratory Fellow and Manager of the Theoretical Materials Science Group before he joined the CSRC in 2015.