复旦大学物理系物质科学报告

Physics Department Colloquium

Band Structure Engineering and Defect Control of Oxides for Energy Applications

Prof. Su-Huai Wei

Beijing Computational Science Research Center

Transition metal and post-transition metal oxides such as ZnO, In_2O_3, SnO_2, TiO_2, and their alloys, play an essential role in modern optoelectronic devices because they have many unique physical properties such as structure diversity, superb stability in solution, good catalytic activity, and simultaneous high electron conductivity and optical transmission. Therefore, they are widely used in energy related optoelectronic applications such as photovoltaics and photoelectrochemical (PEC) fuel generation. In this talk, using first-principles band structure calculations, I will discuss the electronic, optical, and doping properties of oxides and address some fundamental questions related to their unique materials properties such as (i) why most of the transparent conducting oxides (TCOs) are n-type and how to engineer band structure of a transparent oxide so it can be doped both p- and n-type? (ii) Is oxygen vacancy an efficient intrinsic n-type dopant in metal oxides? (iii) To achieve optimal n-type conductivity through extrinsic doping, should we choose dopant substituting on anion site or cation site? (iv) Why amorphous TCO can have good electrical conductivity even without passivation? (v) How to engineer the band structure of oxides through defect control for renewable energy generation?

Time：2:00pm, Tuesday, November 15, 2016

Location：Physics Building, Room 221B

(Cookies and coffee are served from 1:30 pm)