PAP Seminar Announcement

Theoretical Modeling of Electronic, Optical, and Doping Properties of Oxides for Energy Applications

By
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Venue: Hilbert Space (SPMS-PAP-02-02)
Host: Prof. Shen Zexiang

Abstract

Post-transition metal oxides (ZnO, In2O3, SnO2, TiO2, etc.) 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) water splitting. In this work, using first-principles band structure calculations, we will study the electronic, optical, and doping properties of oxides and address some questions related to the unique materials properties of the oxides, including (i) why most of the transparent conducting oxides (TCOs) are n-type and what kind of band structures are good for n-type TCOs? (ii) Are oxygen vacancy an efficient intrinsic n-type dopants (i.e., are the defect levels deep or shallow) 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) Should the doping be done under oxygen-poor or oxygen-rich condition? (v) Why amorphous TCO can have good electrical conductivity even without passivation? And (vi) how to modify the band structure of oxides through defect control for PEC water splitting?

Short Biography

Su-Huai Wei received his B.S. in Physics from Fudan University in 1981 and Ph.D. from the College of William and Mary in 1985. He joined the National Renewable Energy Laboratory in 1985 and is currently a Principal Scientist and Group Manager for the Theoretical Materials Science Group. His research is focused on developing electronic structure theory of materials, especially for semiconductors and energy related materials and applications. He has published more than 340 papers in leading scientific journals, including more than 58 in Physical Review Letters with an H index of 68. He is a Fellow of the American Physical Society.