Metal Halide Perovskites for Next Generation Displays and Solar Cells

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This past decade has seen an unprecedented development in metal halide perovskite -based optoelectronics. Metal halide perovskites share the general formula: ABX_3, in which A, B, and X are occupied by monovalent cations (either organic or inorganic), bivalent metal cations, and halide anions, respectively. Organic-inorganic halide perovskites (OIHPs) in solar cells have achieved close to 24% power conversion efficiencies and all-inorganic halide perovskites (IHPs) have shown over 20% external quantum efficiency in light-emitting diodes (LEDs). Despite this progress, challenges in environmental and operational stability of electronic devices and toxicity issues of lead halide perovskites remain. At a fundamental level, questions pertaining to the structure-property relationship, bulk Rashba effect, and the nature of ferroelectric phenomenon are not completely understood in metal halide perovskites.

In this talk, she will discuss their recent work on the optical properties of cesium lead bromide perovskite ($CsPbBr_3$) nanocrystals (NCs). The incorporation of planar defects greatly enhances the photoluminescence quantum yield and stability against photodegradation. The role of hydrostatic pressure in enhancing the luminescence yield and unraveling structural properties in $CsPbBr_3$ NCs will be discussed. Time permitting, she will discuss their efforts in the synthesis of OIHP films using vapor deposition techniques, which make them air-stable, and their application in solar cells.

Biography

Suchi Guha is a Professor in the Department of Physics and Astronomy at the University of Missouri-Columbia, USA, where she joined as an assistant professor in 2003. She earned her doctorate degree in physics from Arizona State University. Prior to that, she obtained master's and bachelor's degrees in physics from the Indian Institute of Technology, New Delhi and the University of Delhi, respectively. Her current research interests include charge transport mechanisms in polymeric and organic semiconductors, development of organic field-effect transistors and photodetectors, peptide electronics, and photophysics of conjugated polymers and perovskite materials using linear and nonlinear optical spectroscopy. She has co-authored around 120 publications and currently serves as an associate editor of the journal - ACS Applied Electronic Materials.

First-principles calculation of excitonic effects in solids: TDDFT as a low-cost alternative to the Bethe-Salpeter equation

Carsten A. Ullrich, University of Missouri

This talk gives an overview of recent theoretical and computational developments in time-dependent density-functional theory (TDDFT) for periodic insulators and semiconductors. To capture excitonic effects within a TDDFT framework requires exchange-correlation functionals with a proper long-range behavior, which can be efficiently modeled with a class of long-range corrected approximations. While attractive from a computational standpoint, these approximations have their limitations and require judicious use. I will also discuss generalized TDDFT approaches for excitons using a new class of screened hybrid functionals. These represent a cost-efficient alternative to the Bethe-Salpeter equation for the optical properties of solids. Applications to excitonic properties in bulk insulators and semiconductors, including perovskites, will be discussed.

Biographical sketch

Carsten Ullrich received his PhD in Physics from the University of Würzburg, Germany, in 1995, and then had postdoctoral positions in France (Toulouse) and in the US (Missouri, UC Santa Barbara). In 2001 he joined the University of Missouri-Rolla (now Missouri S&T), and moved to the University of Missouri-Columbia in 2005. In 2007 he received tenure, and in 2013 he became a full Professor of Physics. His research expertise is in theoretical and computational condensed-matter physics, with an emphasis on the development of new methodologies within time-dependent density-functional theory (TDDFT). He has around 100 publications, including a textbook on TDDFT (Oxford University Press, 2012). He is a Fellow of the American Physical Society.

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