

Seeing structural origins and foreseeing new pathways to improved functional materials with aberration-corrected STEM

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### Abstract

Structural defects in crystalline materials have been well acknowledged as the major parameters to optimize materials' properties. Controlling and tuning these imperfections can lead to marked improvements in their functional properties. The atomic-scale defects have usually been ignored due to the difficulty of quantifying them via traditional methods. Aberration-corrected scanning transmission electron microscopy (STEM) has developed into the most powerful characterization and even fabrication platform for all materials, especially for functional materials with complex structural features that dynamically respond to external fields. Directly seeing and tuning all scales of defects has now become possible, including the critically important atomic-scale defects. Thoroughly understanding the nature and role of structural defects not only reveals the origin of the structure-property relations of existing high-performance materials, but more importantly, enables us to foresee new pathways to the design of new materials with enhanced properties.

In my thesis, I will show the achievements and new insights obtained from representative functional materials, including piezoelectrics/ferroelectrics, functional oxide interfaces, thermoelectrics, and electrocatalysts. STEM probe imaging was used for investigation into the quantitative atomic displacements of local polarization states in the rapidly evolving field of piezoelectric ceramics, where significant advance is being made to unveil the complex phase boundaries and physical origin of the remarkable piezoelectric properties. We can also visualize both intrinsic and extrinsic defects at the atomic scale, which are shown to play a dominant role in thermal and electrical transport properties, comparable to the widely accepted role of nanostructuring. The same applies to electrocatalysts, where various defects down to the atomic scale have led to much improved electrochemical performance. We highlight a universal strategy to optimize the properties of these functional materials, atomic-scale defect engineering.

Mr. WU Haijun is now a PhD student of Prof. Stephen John Pennycook. His present research interests are scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS), and the structural-property correlation of energy materials, including functional oxides (e.g., ferroelectric/ferromagnetic/ferroelastic materials), and semiconductors (e.g., thermoelectric materials). He got the bachelor and master degrees from Xi'an Jiaotong University, China in 2009 and 2012 respectively. After graduation, He worked as TEM engineer at Xi'an Jiaotong University and South University of Science and Technology for three years.

## WU Haijun

# Speaker Wu Haijun

### **Prof Ding Jun Host**