50-Year Old Physics Problem Resolved at Southern University

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RII: Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA)
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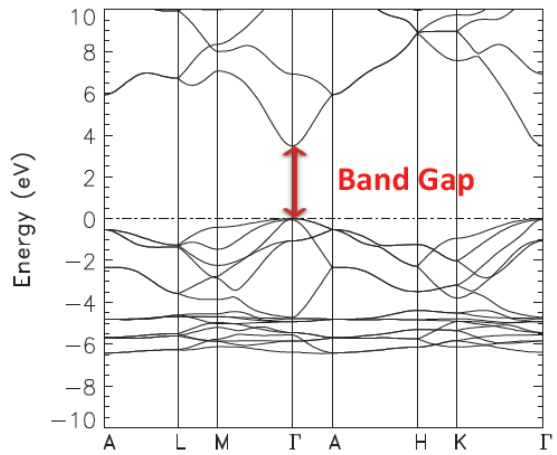
PI: Dr. Michael Khonsari

What is the outcome or accomplishment?
A team of LA-SiGMA researchers at Southern University led by Dr. Diola Bagayoko has mathematically resolved a 50-year old physics problem: how to calculate the accurate measured band gap of semiconductor and insulator materials. The equations used in the physics field of density functional theory over the last half century have systematically underestimated the band gap.

What is the impact?
This resolution ushers in an era of highly accurate description and prediction of properties of materials and has profound implications for condensed matter theory and direct applications in electronic industry, nanoscience and technology, and particularly in the U.S. Materials Genome Initiative.

What explanation/background does the lay reader need to understand the significance of this outcome?
Forces are created by electrons and atoms, which together influence the quantum mechanical behaviors of electrons in many different ways, making predictive calculations difficult.



The double-headed arrow in this energy diagram for zinc oxide (ZnO) represents the calculated band gap that agrees with experiments. Zinc oxide is a compound used for many applications, including sunscreen and rubber. It has a wide direct band gap at room temperature, so it has potential as a material for future electronics.

Credit: Dr. Diola Bagayoko, Southern University and A&M College, diola_bagayoko@subr.edu

The band gap is the smallest width of the “forbidden” range of energy between the levels that are empty and the levels that are occupied by electrons. In the diagram, the occupied energies are represented by the lines below zero while the empty ones are above zero. The double-headed arrow represents the band gap.

Accurate prediction of the band gap is of critical importance for numerous properties and applications of semiconductors and insulators. A rigorous, mathematical understanding of density functional theory and the completion of this theory in practice made the above solution possible. Consequently, Dr. Bagayoko’s team has correctly predicted the band gaps and other properties of over 30 semiconductors.