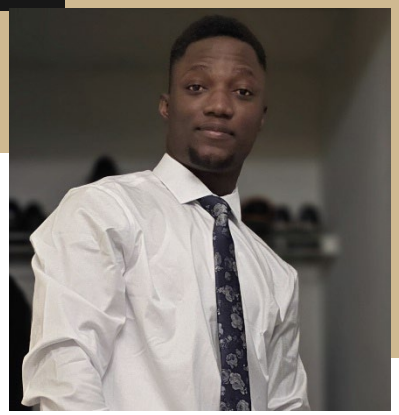
INORGANIC SEMINAR



Emmanuel Adeniyi

Graduate Student | Andrews Group | Purdue University

High Capacity but at What Cost? Irreversible Formation of "Hidden" Molecular Oxygen in Li-Rich Cathodes

Lithium-ion batteries are widely used for portable electronics, electric vehicles, and grid-level energy storage, but their energy density is limited by the capacity of conventional transition-metal (TM) oxide cathodes. Common cathode materials such as $LiCoO_2$ and $LiFePO_4$ store charge primarily through transition metal redox reactions, which restrict the amount of lithium that can be reversibly removed from the structure. To overcome this limitation, so-called "Li-rich" layered oxides cathode materials have been developed. In principle, these materials can deliver higher capacities by invoking both transition-metal and oxygen redox processes.

"Li-rich" materials such as $Li_{1.2}Ni_{0.13}Co_{0.13}Mn_{0.54}O_2$ exhibit capacities far above those of conventional cathode materials, making them attractive candidates for next generation high energy-density batteries. However, the extra capacity afforded by oxygen oxidation is accompanied by several challenges, including voltage fade, irreversible capacity loss, and structural instability during cycling. Recent spectroscopic studies have shown that these effects are associated with the formation of molecular oxygen within the bulk of the cathode during charging. Some of this "hidden" O_2 remains trapped in the structure and leads to irreversible and deleterious changes in local TM-oxygen bonding environment that ultimately degrade electrochemical performance.

In this seminar, I will review the operating principles of lithium-ion batteries and discuss the limitations of conventional cathode materials such $LiCoO_2$. I will also introduce Li-rich layered oxides, with emphasis on $Li_{1.2}Ni_{0.13}Co_{0.13}Mn_{0.54}O_2$ and explain how oxygen redox contributes to their high capacity. Finally, I will discuss recent experimental evidence for the irreversible formation of molecular oxygen in these materials and evaluate the trade-off between achieving high capacity and maintaining structural stability in Li-rich cathodes.

PURDUE UNIVERSITY | James Tarpo Jr. and Margaret Tarpo Department of Chemistry

Tuesday, April 7, 2026 | 12:30 PM | BRWN 4102

INORGANIC SEMINAR

Kaixin Wu

Graduate Student | Andrews Group | Purdue University

2D Conductive Metal–Organic Frameworks in Thermoelectrics

Thermoelectric materials can directly convert thermal energy into electrical energy, making them attractive for recovering energy that is lost as heat, known as “waste heat.” High thermoelectric efficiency is achieved by maximizing the so-called “figure of merit” (ZT), which depends on the Seebeck coefficient, electrical conductivity, and thermal conductivity of a given material. As a first approximation, ZT is highest when electrical conductivity is high and thermal conductivity is low. Traditional inorganic thermoelectric materials often have limitations such as toxicity, rigidity and high cost, which has prompted the exploration of alternative systems. The emergence of two-dimensional electrically conductive metal-organic frameworks (2D c-MOFs) generated interest in their use as thermoelectric materials. Metal-organic frameworks (MOFs) possess unique advantages. 2D c-MOFs exhibit enhanced charge transport performance due to their extended π-conjugated networks and layered structures and yet because they are mostly empty space, they also possess inherently low thermal conductivity. Recent studies in this area have investigated 2D c-MOF materials, such as $Cu_3(HHTP)_2$ and $Li_xFe_3(HTTP)_2$, for application as thermoelectrics. In this seminar, I will highlight several of these studies, including a recent report on the use of Ni-BHT that has a theoretically calculated ZT value of 0.92. Despite these advancements, the ZT values of MOF-based thermoelectric materials are still lower than those of traditional solid state systems due to their limited electrical conductivity. I will discuss approaches to improving these materials, including strategies such as molecular design, doping, and composite formulation.

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