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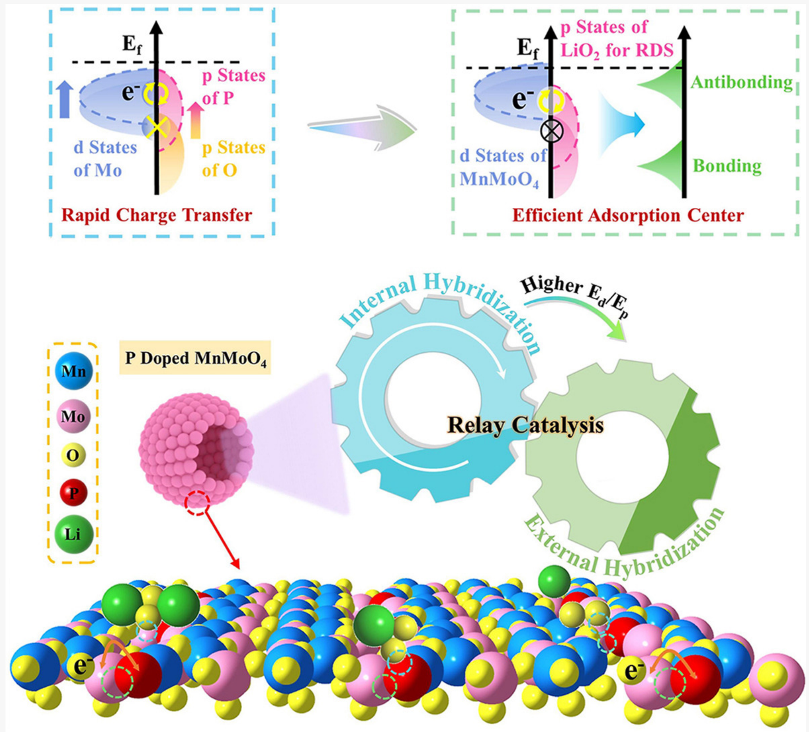
New catalyst design boosts stability and efficiency of lithium–oxygen batteries

GA, UNITED STATES, August 22, 2025 /EINPresswire.com/ -- Lithium–oxygen batteries (LOBs) offer extraordinary energy density but face critical roadblocks in efficiency and lifespan. A new study unveils a breakthrough catalyst design using phosphorus-doped MnMoO4 hollow nanospheres, which leverage a "relay orbital hybridization" effect to accelerate reaction kinetics and stabilize cycling. This approach strengthens internal bonding within the catalysts while simultaneously activating external orbital interactions with lithium superoxide intermediates, dramatically improving charge transfer. As a result, the engineered cathodes delivered stable operation for over 380 cycles at high current density, outperforming even some noble-metal systems. The discovery provides a blueprint for designing cost-effective catalysts capable of powering the next generation of sustainable energy storage.



Relay Orbital Hybridization Boosts Lithium–Oxygen Battery Catalysis.

The urgency of the global energy transition calls for batteries that surpass the capacity of conventional lithium-ion systems. LOBs are especially promising, offering nearly ten times higher theoretical energy density. Yet, their widespread use has been held back by poor conductivity, high overpotentials, and rapid performance decay, all stemming from sluggish oxygen reactions. MnMoO4, a stable and abundant transition metal oxide, holds potential as a cathode catalyst, but its weak interaction with oxygen intermediates has restricted electrocatalytic property. Due to these challenges, researchers sought to develop orbital-level engineering strategies to unlock MnMoO4's catalytic activity and extend the lifespan of LOBs.

In a study published June 18, 2025, in eScience, scientists from Shandong University and the

University of Adelaide introduced a phosphorus-doped $MnMoO_4$ catalyst that dramatically improves LOB performance. By inducing a relay orbital hybridization effect—where internal Mo–P interactions activate external coupling with oxygen intermediates—the team achieved unprecedented durability and efficiency. Their optimized cathodes sustained more than 380 cycles at a high current density of 1000 mA g^{-1}, surpassing traditional $MnMoO_4$ and rivaling noble-metal catalysts. This innovation offers a new path toward practical high-energy storage devices.

To tackle the limitations of $MnMoO_4$, the researchers designed hollow nanospheres doped with phosphorus atoms, combining density functional theory (DFT) simulations with experimental synthesis. The doping introduced strong orbital hybridization between Mo 4d and P 3p states, shifting the d-band center and significantly improving conductivity. This internal modification then activated external orbital interactions with LiO_2 intermediates, lowering reaction barriers and accelerating charge transfer. Structural analysis confirmed lattice expansion, uniform phosphorus incorporation, and abundant oxygen vacancies, creating more active sites for catalysis. Electrochemical tests revealed that the optimized 0.75P- $MnMoO_4$ cathode delivered a remarkable specific capacity above 13,000 mAh g^{-1} with Coulombic efficiency over 95%. Most strikingly, it maintained stable cycling for more than 380 cycles under high current densities, far outperforming undoped $MnMoO_4$ and other state-of-the-art oxide cathodes. Demonstrating practical application, a pouch-type lithium–oxygen cell powered LED arrays for more than 560 hours. The combination of orbital-level tuning and nano-architecture highlights a transformative strategy for creating low-cost, high-performance catalysts.

"By strategically introducing phosphorus atoms, we unlocked a relay hybridization effect that redefines how $MnMoO_4$ interacts with oxygen intermediates," said Associated Professor Jun Wang and Professor Zaiping Guo, co-corresponding authors of the study. "This approach enhances intrinsic conductivity and optimizes reaction pathways, allowing LOBs to operate with far greater stability and efficiency. Importantly, the strategy is scalable and cost-effective, showing that we can rival noble-metal systems without their expense. Our findings provide a guiding principle for the rational design of catalysts across clean energy technologies."

The advance of phosphorus-doped $MnMoO_4$ catalysts represents more than a step forward for LOBs—it marks a paradigm shift in how catalysts can be designed for sustainable energy storage. The improved cycling stability and high efficiency pave the way for batteries capable of supporting renewable energy grids, long-range electric vehicles, and portable electronics with extended lifespans. Beyond LOBs, the relay orbital hybridization concept may also be applied to other critical systems, such as zinc–air batteries, hydrogen production, and CO_2 conversion. By bridging fundamental orbital chemistry with real-world performance, this study opens the door to scalable, next-generation power technologies.

References

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