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Formation of small polarons in Li_2O_2 and implications for Li-air batteries[1] JOONGOO KANG, National Renewable Energy Laboratory, Golden, Colorado 80401, USA, YOON-SEOK JUNG, Ulsan National Institute of Science and Technology, Ulsan, Korea, SUHUAI WEI, ANNE DILLON, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — Lithium-air batteries (LABs) have recently been revitalized as a promising electrical energy storage system due to their exceptionally high theoretical energy density. However, its usage is limited by poor rate capability and large polarization in the cell voltage due primarily to the formation of Li_2O_2 in the air cathode. Here, using hybrid density functional theory, we found that the formation of small polarons in Li_2O_2 is the origin that limits the electron transport in Li_2O_2. Consequently, the low electron mobility contributes to the hysteresis in cell voltage and limits the power density of the LABs. We suggest that similar behavior should exist in other peroxides, and p-type doping in Li_2O_2 could significantly improve the performance of LABs at high current densities.

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