Lewis Acidity Modified Heme Molecular Catalysts for Lithium-Oxygen Battery

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As the commercialization of the electric vehicles, the lithium-oxygen batteries have attracted attention for its high theoretical specific energy of 3458 W h kg^{-1}. Nevertheless, the practical use of the lithium-oxygen batteries has encountered hindrance owing to the low cycle life and large overpotential. While various catalysts such as metal oxides and metal nanoparticles were applied to the air-cathode to ameliorate overpotential and cyclability, designing effective catalysts is still challenging. Inspired by the oxygen scavenging effect of the hemoglobin, herein, we synthesized the ligand modified heme catalysts for air-cathode in which the electron-withdrawing ligands such as thiocyanate(NCS^-) and azide (N_3^-) were coordinated to the Fe center. The enhanced lewis acidity induced weaker binding of the oxygen intermediate (O_2^*) resulting in facile decomposition of Li_2O_2. Density functional theory calculation together with the surface energy analysis support the effect of the ligand modified catalysts in enhancing $Li-O_2$ battery reversibility.