New strategy for cathode materials in lithium-chlorine battery

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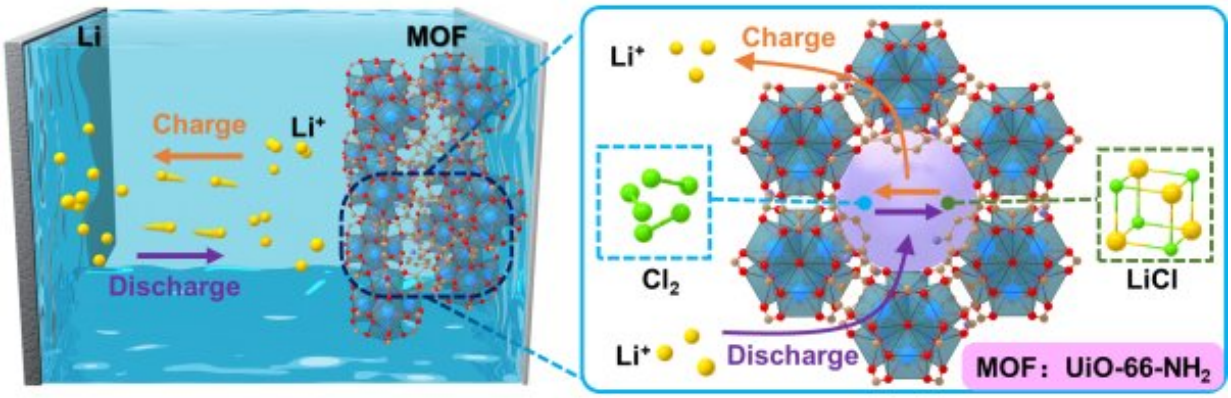

The schematic diagram of the reaction mechanism of Li-Cl_2@MOF(UiO-66-NH_2) batteries. Credit: Xu Yan et al

A team led by Prof. Chen Wei, Prof. Jiang Hailong and Prof. Li Zhenyu from the University of Science and Technology of China (USTC) adopted NH_2-functionalized metal-organic frameworks (MOFs) in lithium-chlorine (Li-Cl_2) batteries to achieve high specific capacities, cycle stability and superior low-temperature performance. Their work was published in *Joule* on March 15.

Traditional lithium-thionyl chloride (Li-$SOCl_2$) batteries are widely used for their high energy density and other advantages, but alternatives are still needed since Li-$SOCl_2$ batteries are not rechargeable. Rechargeable

Li-Cl_2 battery was first invented in 2021, with a high specific capacity of 1200 mAh/g and a high output voltage of ~3.6 V.

However, the following problems stand in the way of the practical application of Li-Cl_2 battery. First, the Cl_2 reaction is limited by the weak physical adsorption of porous carbon to Cl_2 molecules. Second, the excessive LiCl generation into the carbon pores blocks the channels for Li^+ transportation and Cl_2 diffusion, hindering further electrochemical reactions. Furthermore, the shuttle effect of unbonded Cl_2 leads to battery capacity decay, especially at high output capacities. Therefore, the cathode materials with highly porous structures are vital to realize high-performance Li-Cl_2 batteries.

To overcome these difficulties, the team proposed that MOFs with Lewis basic functional groups should be applied to improve the cathode Cl_2/LiCl reactions. Guided by theoretical predictions, MOFs with -NH_2 functional groups were screened out using first-principles calculation and applied in Li-Cl_2 batteries. Cryo-TEM and low-dose high-resolution TEM showed that UiO-66-NH_2 maintains a very stable structure during cycling, and XPS verified -NH2 groups' strong affinity to Cl_2 and LiCl, thus enhancing its redox reaction kinetics. Li-Cl_2@MOF batteries designed by the team reached a maximum discharge specific capacity of 2000 mAh/g and are stable for more than 500 cycles at a specific capacity of 1000 mAh/g. Meanwhile, the batteries performed stable function under the temperature of -40°C.

More information: Yan Xu et al, Metal-organic frameworks for nanoconfinement of chlorine in rechargeable lithium-chlorine batteries, *Joule* (2023). DOI: 10.1016/j.joule.2023.02.010

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