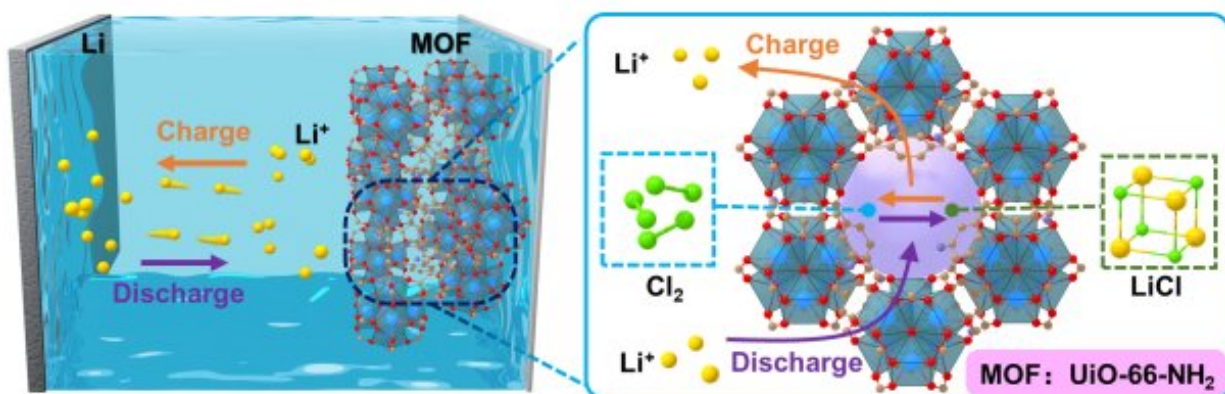


# New strategy for cathode materials in lithium-chlorine battery

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The schematic diagram of the reaction mechanism of Li-Cl<sub>2</sub>@MOF(UiO-66-NH<sub>2</sub>) 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<sub>2</sub>-functionalized metal-organic frameworks (MOFs) in lithium-chlorine (Li-Cl<sub>2</sub>) 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<sub>2</sub>) batteries are widely used for their [high energy density](#) and other advantages, but alternatives are still needed since Li-SOCl<sub>2</sub> batteries are not rechargeable. Rechargeable

Li-Cl<sub>2</sub> 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<sub>2</sub> battery. First, the Cl<sub>2</sub> reaction is limited by the weak physical adsorption of porous carbon to Cl<sub>2</sub> molecules. Second, the excessive LiCl generation into the carbon pores blocks the channels for Li<sup>+</sup> transportation and Cl<sub>2</sub> diffusion, hindering further electrochemical reactions. Furthermore, the shuttle effect of unbonded Cl<sub>2</sub> 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<sub>2</sub> batteries.

To overcome these difficulties, the team proposed that MOFs with Lewis basic functional groups should be applied to improve the cathode Cl<sub>2</sub>/LiCl reactions. Guided by theoretical predictions, MOFs with [-NH<sub>2</sub> functional groups](#) were screened out using first-principles calculation and applied in Li-Cl<sub>2</sub> batteries. Cryo-TEM and low-dose high-resolution TEM showed that UiO-66-NH<sub>2</sub> maintains a very stable structure during cycling, and XPS verified -NH<sub>2</sub> groups' strong affinity to Cl<sub>2</sub> and LiCl, thus enhancing its redox reaction kinetics. Li-Cl<sub>2</sub>@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](https://doi.org/10.1016/j.joule.2023.02.010)

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