## 发表文章中仪器标注

**1.简版：**

**标注仪器型号，生产厂家和使用的单色器及电压电流值（标黄部分请根据实际情况修改）**

X-ray absorption fine structure (XAFS) spectroscopy was carried out using the *RapidXAFS* HE (Anhui Absorption Spectroscopy Analysis Instrument Co., Ltd.) by transmission mode at 20 kV and 20 mA,

 and the **Si (733)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Zn or Hf**.

the **Si (533)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Co**

the **Si (771)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Pt or Au**

the **Si (553)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Cu**

the Ge **(310)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Fe**

the **Si (551)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Ni**

the **Si (440)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Mn**

the **Si (664)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Ir**

the **Si (110)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Mn Ta Bi or Pb**

the **Ge (111)** spherically bent crystal analyzer with a radius of curvature of 500 mm was used **for Dy or Br**

**详细版：标黄部分请根据实际情况修改**

In this investigation, both static and in-situ X-ray absorption fine structure (XAFS) analyses of the Cu K-edge were conducted utilizing a commercial Laboratory-Based XAFS spectrometer (RapidXAFS HE, Anhui Absorption Spectroscopy Analysis Instrument Co., Ltd.). X-rays were generated via a Mo (or W) target X-ray source operated at 20 kV and 20 mA. A Si (553) spherically bent crystal analyzer (SBCA) with a radius of curvature of 500 mm served as the monochromator, thereby ensuring a diffraction geometry approaching a 90-degree backscatter angle at the absorption edge. After monochromatization, the X-rays pass through the sample and were collected using a high-energy-resolution silicon drift detector (SDD) to obtain the X-ray intensity. The XAFS data were acquired in transmission mode. During the XAFS measurements, the position of the absorption edge (E0) was calibrated using a standard Cu foil sample, and all data collection occurred within a single time period.

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X-ray absorption fine structure (XAFS) spectroscopy was carried out using the RapidXAFS HE Ultra by transmission mode at 20 kV and 20 mA, and the Si (551) spherically bent crystal analyzer with a radius of curvature of 500 mm was used for Ni; the Si (553) spherically bent crystal analyzer with a radius of curvature of 500 mm was used for Cu; the Si (771) spherically bent crystal analyzer with a radius of curvature of 500 mm was used for Pt. The obtained XAFS data was processed in Athena (version 0.9.26) for background, pre-edge line and postedge line calibrations. Then Fourier transformed fitting was carried out in Artemis (version 0.9.26). The k3 weighting, k-range of 2- 9 Å−1 and R range of 1.2 −3 Å were used for the fitting. The four parameters, coordination number, bond length, Debye-Waller factor and E0 shift (CN, R, σ2, ΔE0) were fitted without anyone was fixed, constrained, or correlated.

**以下是原位测试可以补充的内容参考：**

**A 电催化**

For the electrochemical in situ XAFS tests, a custom-made cell was utilized, the Cu sample is uniformly dispersed on carbon paper and immersed in a 0.5 M KOH electrolyte. XAFS spectra were acquired through the transmission mode. To track the evolution of the active site during the electrochemical reaction, a range of representative potentials (1.25–1.45 V) were applied to the electrode. This comprehensive approach provides valuable insights into the structural changes of the Cu K-edge during electrochemical reactions.

**B 热催化**

For the thermocatalysis in situ XAFS tests, a custom-made cell was utilized. Catalyst powder was compressed into thin discs and subsequently mounted in the cell holder. XAFS spectra were acquired through the transmission mode. To track the evolution of the active site during the thermocatalysis reaction, the catalyst was heated from room temperature to 300 °C under 5 vol. % H2 in He atmosphere to avoid any oxidation. This comprehensive approach provides valuable insights into the structural changes of the Co K-edge during thermocatalysis reactions.

**C 软包电池**

For the in-situ X-ray absorption fine structure (XAFS) tests conducted on Lithium-ion batteries (LIBs), all charging and discharging operations were executed using a LAND Battery Testing System, model CT2001A 5V1A, from Wuhan LAND Electronics Co., Ltd. Charging and discharging were conducted at C/5 rates across the Ni, Co, and Mn K-edges employing a nominal 4 mA current. Nominal charge rates were computed based on an ideal capacity of 20 mAh. During all in-situ XANES experiments, the cycle commenced with an approximate 10-minute rest period, followed by a discharge at C/5 to 2.7 V, a 5-minute pause, charging at the appropriate rate to 4.3 V, a 5 min pause, discharge at the appropriate rate to 2.7 V, and concluded with another rest period lasting approximately 10 minutes. This meticulous methodology offers profound insights into the oxidation state and structural changes of LIBs throughout the charge and discharge processes.