Supporting information

Script S1

```
# Install and load the 'ade4' package for PCA and HCA analysis

install.packages("ade4")

library(ade4)



# Install and load the 'readxl' package to read Excel files

install.packages("readxl")

library(readxl)



# Install and load the 'MASS' package for discriminant analysis

install.packages("MASS")

library(MASS)



# Read data from an Excel file with XRF spectra data of 108 batteries

data <- read_excel("File name.xlsx")



# Perform PCA (Principal Component Analysis) on the dataset

pca_result <- dudi.pca(data[, -1], scannf = FALSE, nf = 2)
```

```
# Extract the first two principal components

pc1 <- pca_result$li[,1]

pc2 <- pca_result$li[,2]



# Perform hierarchical clustering on the PCA results

hca_result <- hclust(dist(pca_result$li[,1:2]))



# Plot the dendrogram of the hierarchical clustering

plot(hca_result)



# Define a range of heights to evaluate the number of groups

heights <- seq(0, 7, by = 0.1)

num_groups <- sapply(heights, function(h) length(unique(cutree(hca_result, h = h))))



# Select a height that results in exactly 5 groups

selected_height <- heights[which(num_groups == 5)[1]]



# Add a red dashed line to the dendrogram at the selected height

abline(h = selected_height, col = "red", lty = 2)
```

```
# Cut the dendrogram into groups based on the selected height
groups <- cutree(hca_result, h = selected_height)

# Print the group assignments for each sample
print(groups)

# Assign meaningful names to the groups (e.g., "a", "b", "c", "d", "e")
group_names <- c("a", "b", "c", "d", "e")
group_labels <- group_names[groups]

# Create a dataframe with sample names and their corresponding group labels
result <- data.frame(data[,1], group_labels)

# Print the samples in each group
for (group_name in group_names) {
  cat("Group", group_name, ":", paste(result[result$group_labels == group_name, 1], collapse
= ", "), "\n")
}

# Read XRF spectra data of new batteries for classification
```

```
new_data <- read_excel("new data file name.xlsx")


# Extract feature variables and target variable

X <- data[, -1]  # Feature variables

y <- as.factor(group_labels)  # Target variable


# Train the discriminant analysis model

discriminant_model <- lda(X, y)


# Use the discriminant analysis model to predict new data

predicted_groups <- predict(discriminant_model, newdata = new_data[, -1], type = "posterior")


# Combine sample names and prediction results

predicted_result <- data.frame(Sample = new_data[,1], Group = predicted_groups$class)


# Print the prediction results

print(predicted_result)

print(predicted_groups)
```

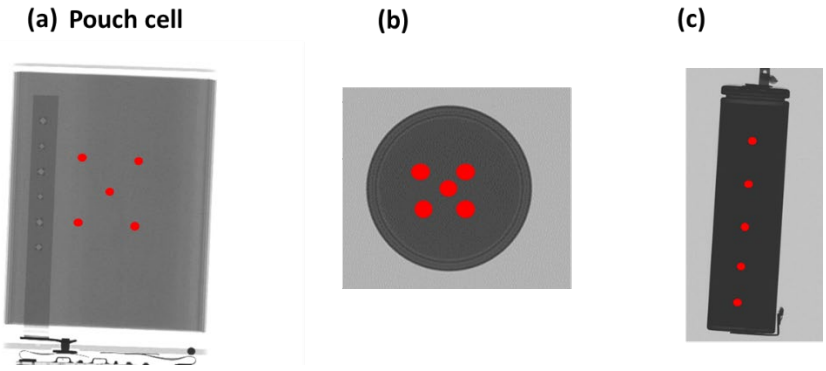

Figure S1. XRT image of (a) pouch cell, (b) coin cell and (c) cylindrical cell marking five X-ray focusing points for XRF experiments.

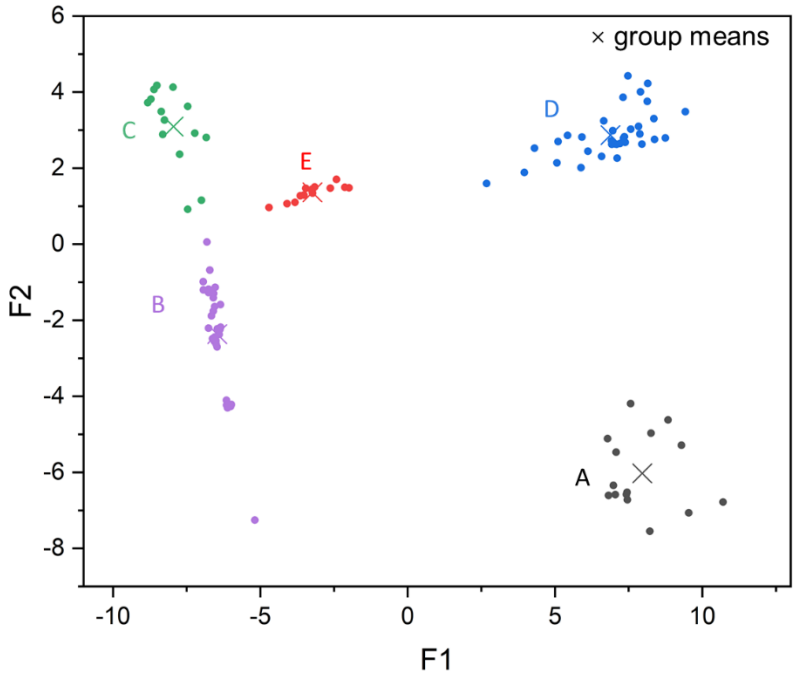

Figure S2. Discriminant function Plot of the 108 batteries.

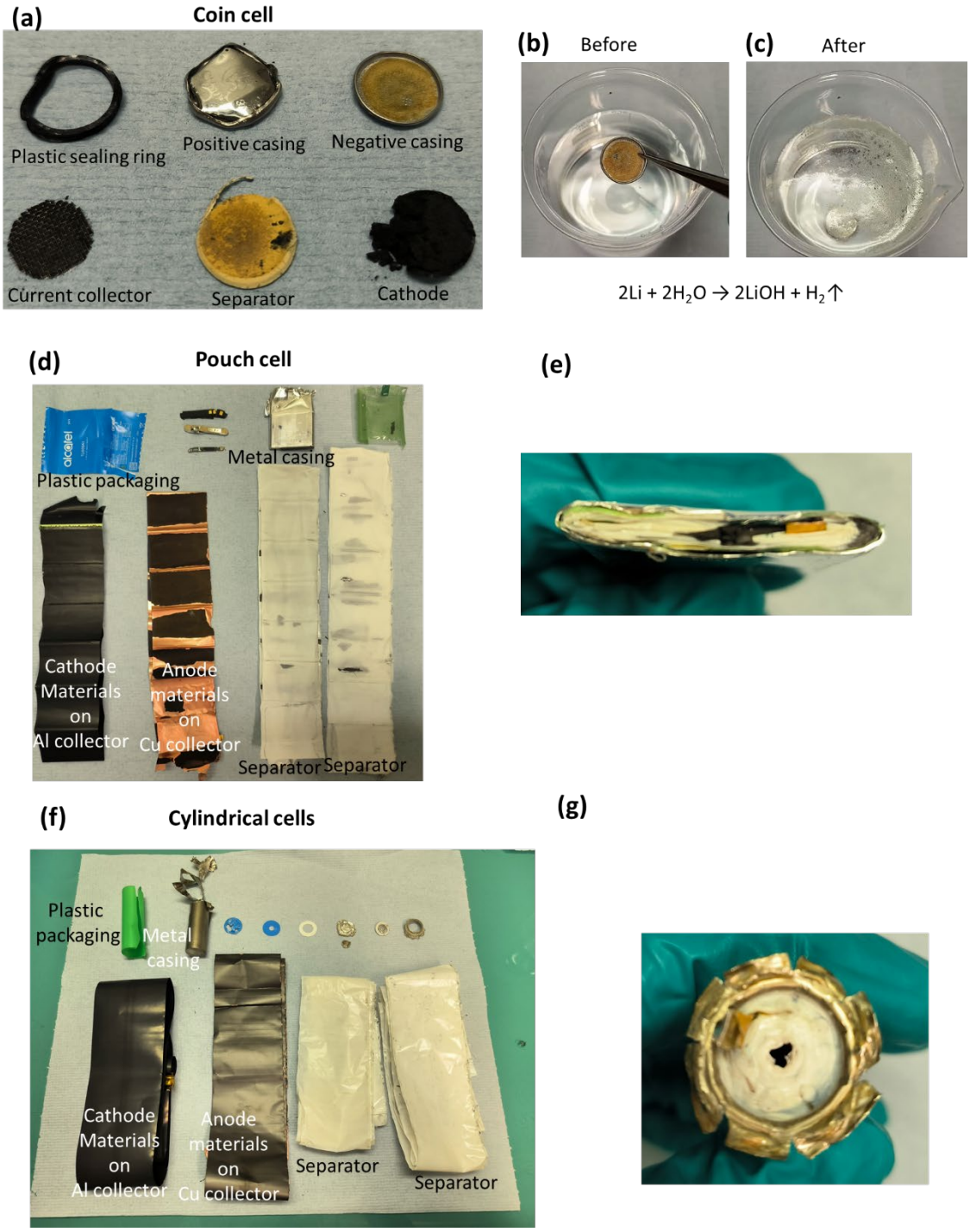

Figure S3. Components of disassembled (a) coin cell, (b) pouch cell and (c) cylindrical cell; Negative casing of coin cell (b) before and (c) after put in the water; Cross-sectional view of disassembled (e) pouch cell and (g) cylindrical cell.

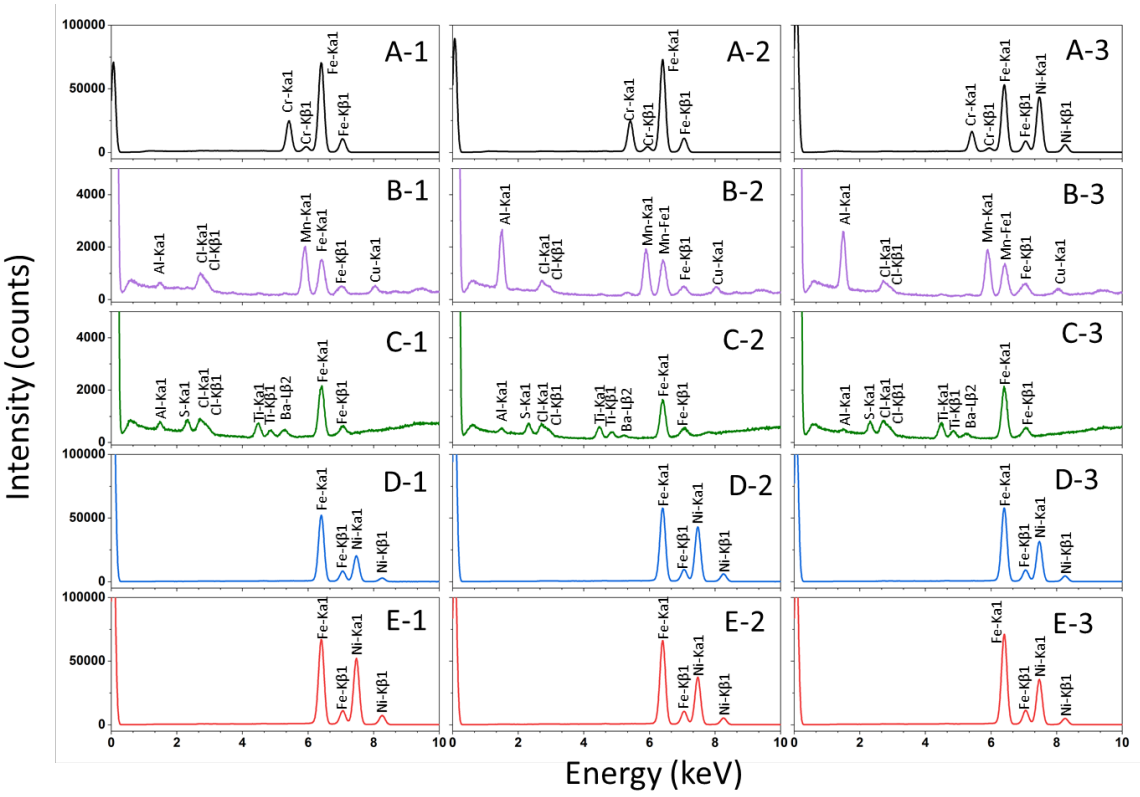

Figure S4. XRF spectra of metal casing of 15 samples from 5 groups (3 samples from each groups).

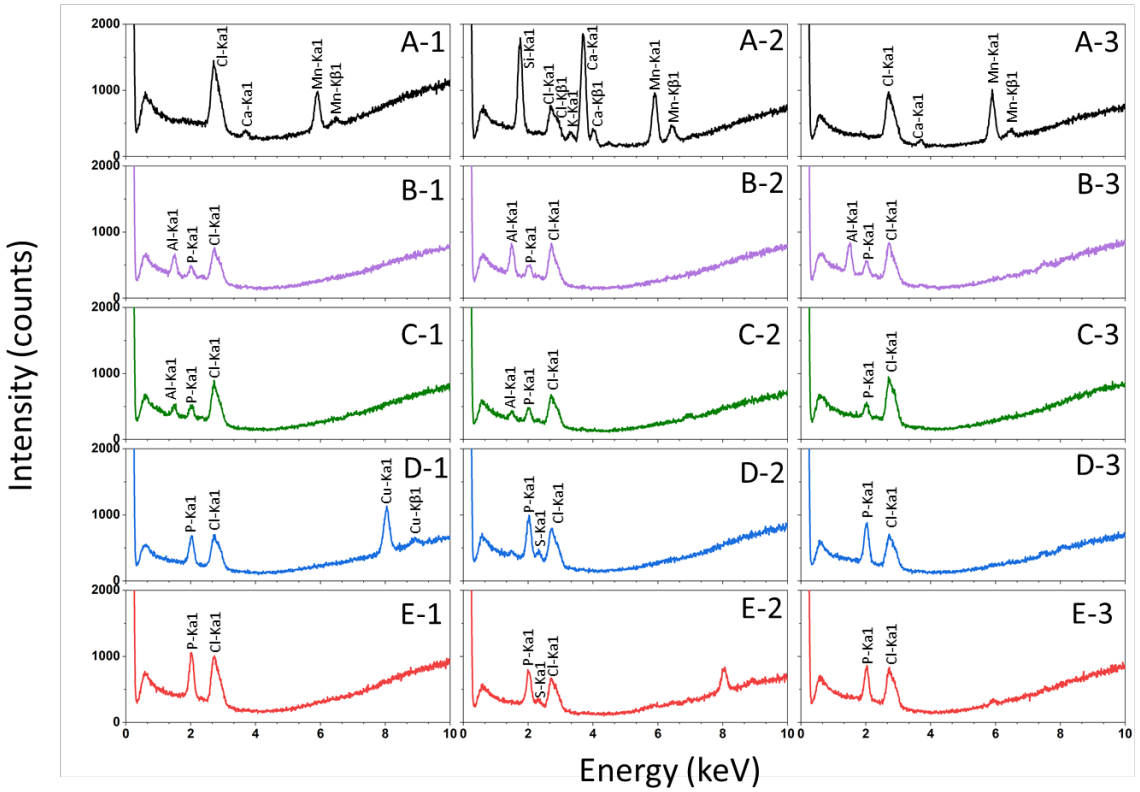

Figure S5. XRF spectra of separator of 15 samples from 5 groups (3 samples from each groups).

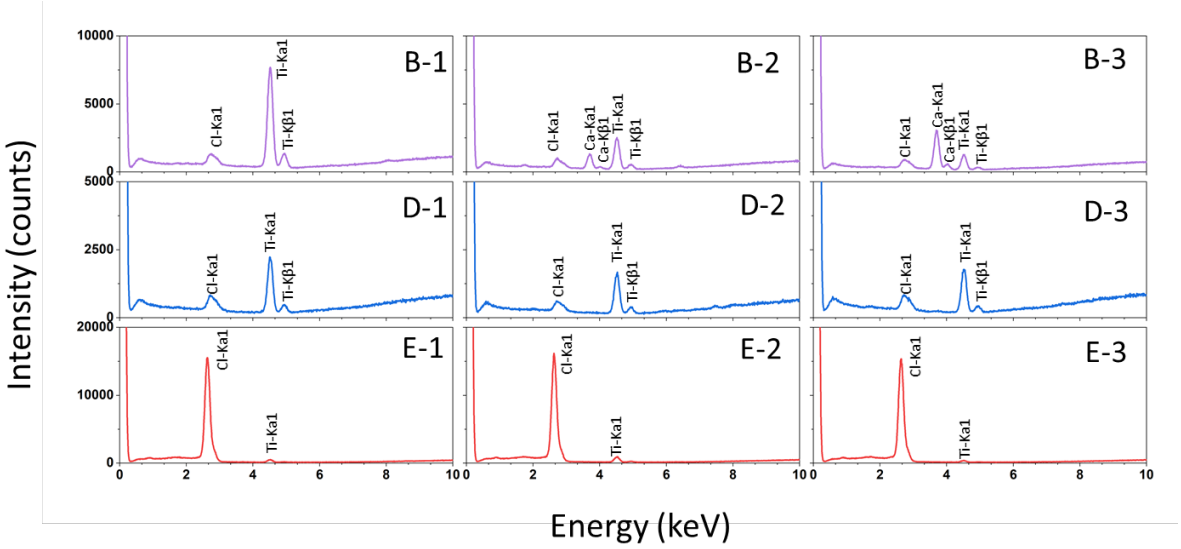

Figure S6. XRF spectra of plastic packaging of 9 samples from group B, D and E.

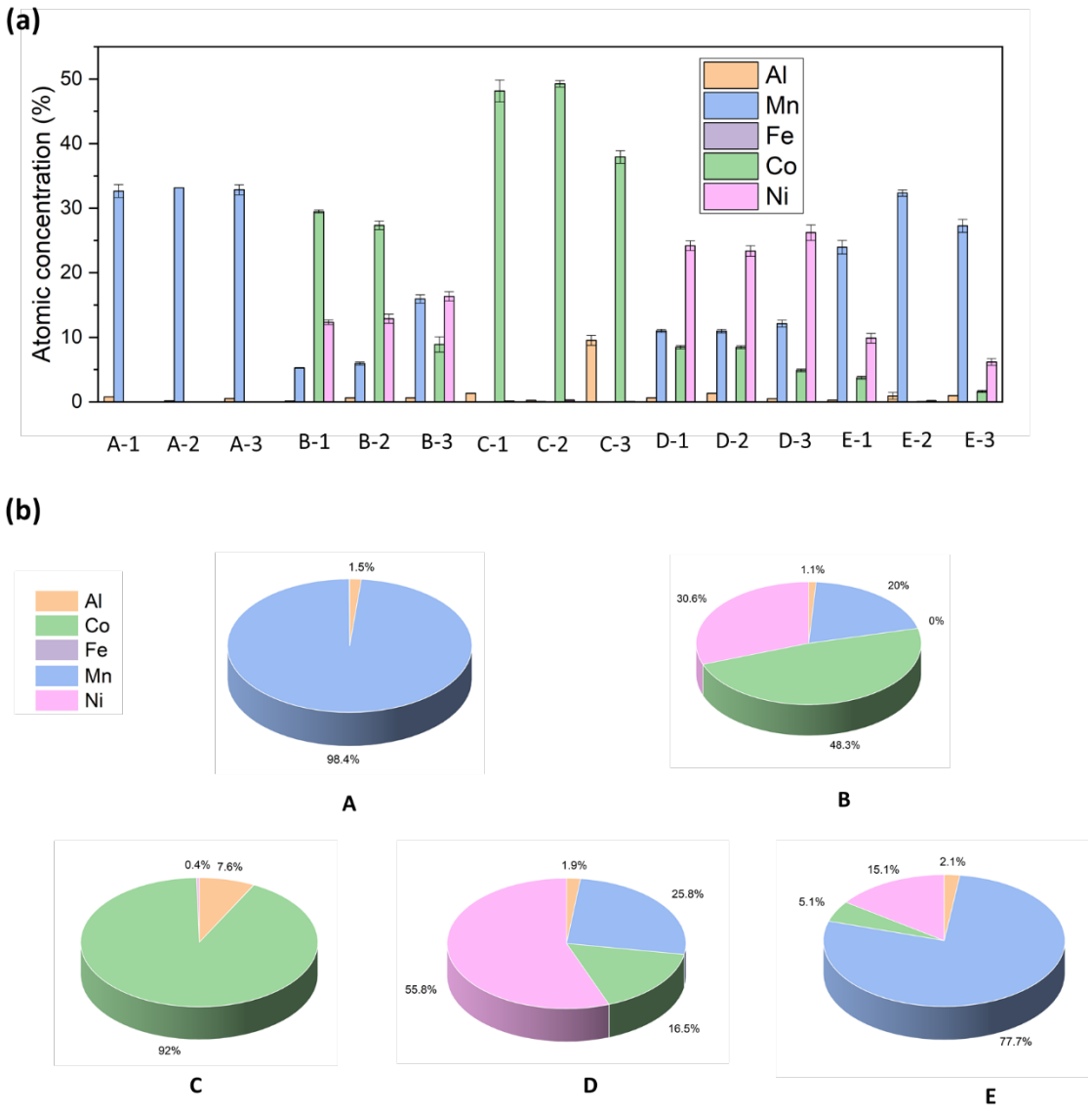

Figure S7. Semi-quantity analysis from XRF: (a) atomic concentration of elements Al, Mn, Fe, Co, and Ni in each group; (b) average atomic concentration of elements in each group.

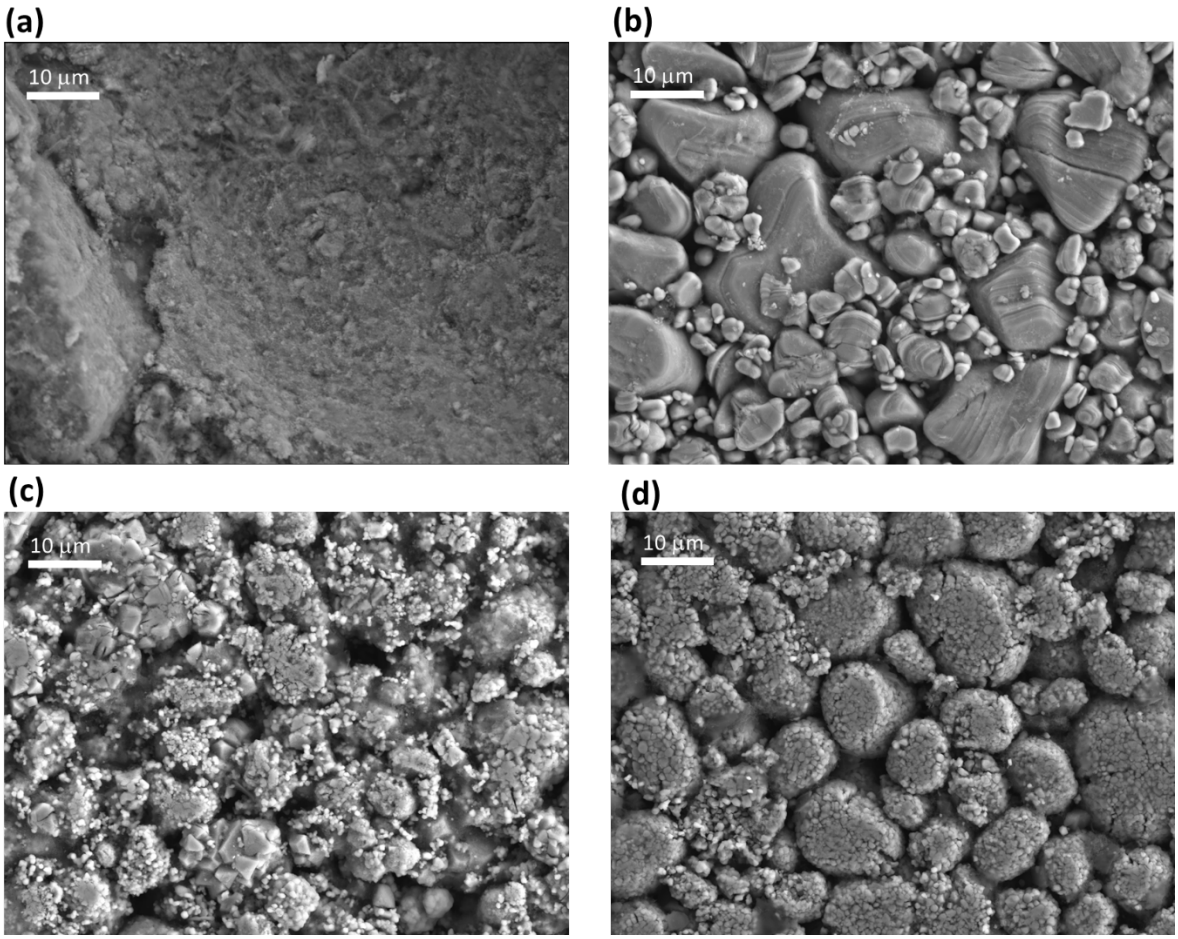

Figure S8. SEM images of (a) A-2, (b) C-1, (c) E-2, and (d) D-1.

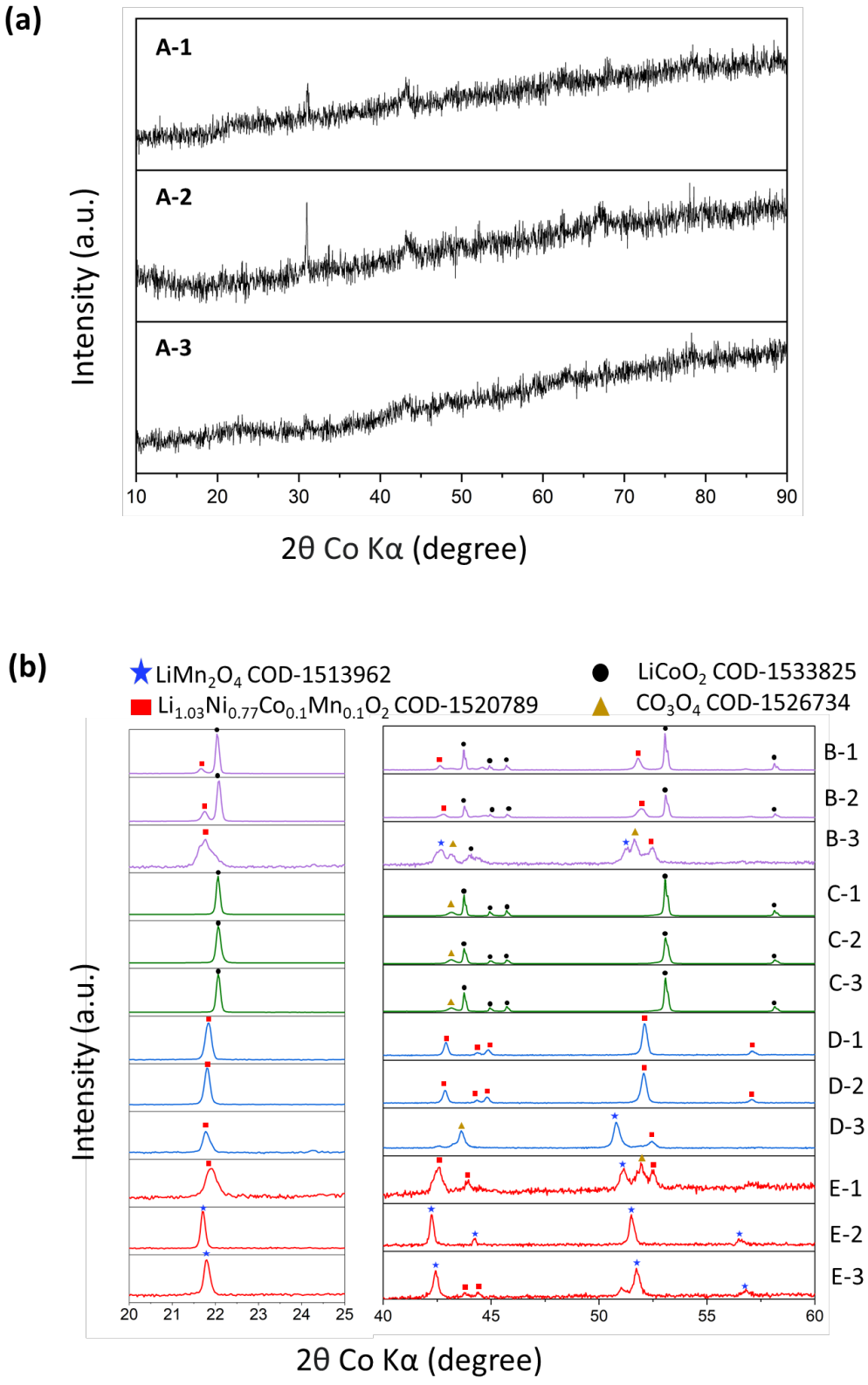

Figure S9. XRD spectra of (a) group A and (b) group B, C, D and E.

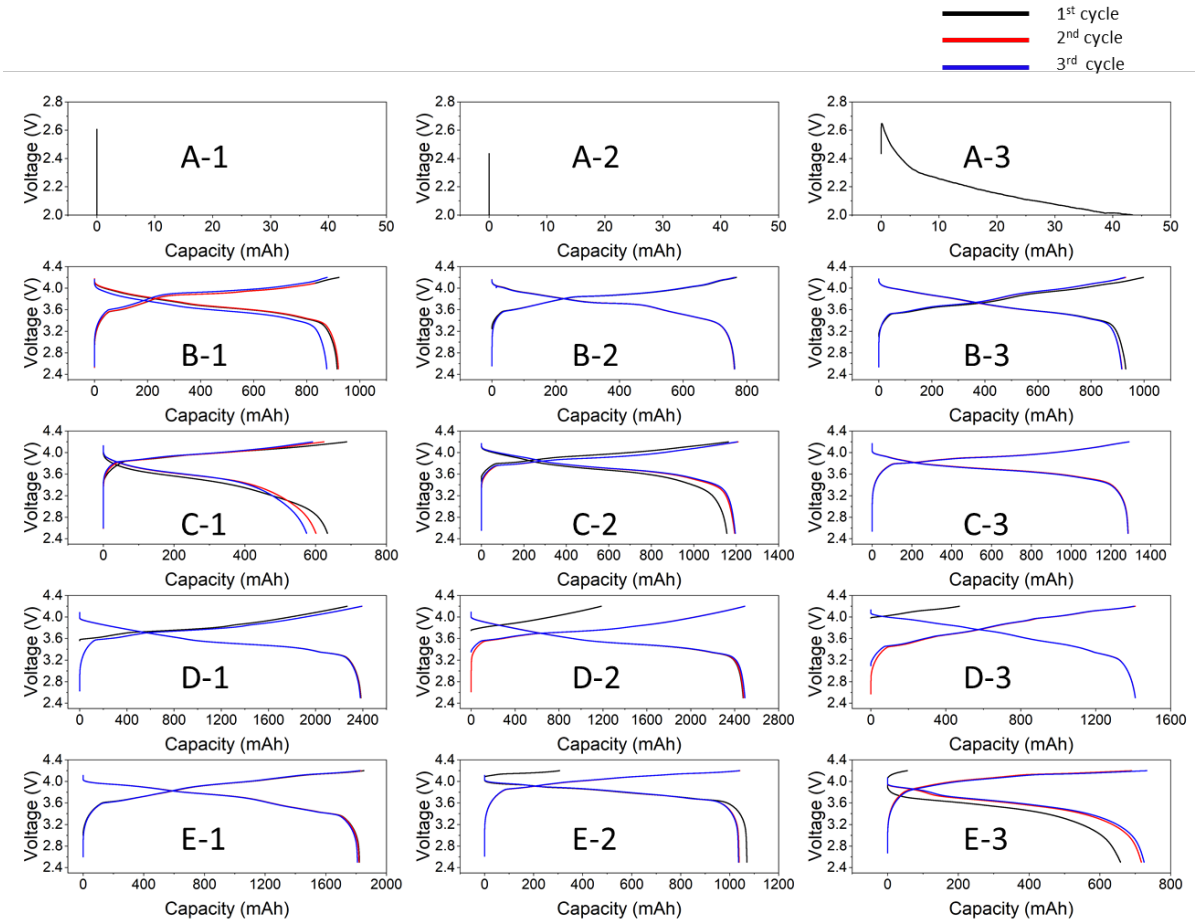

Figure S10. Discharge-charge curves of 15 batteries from 5 groups.

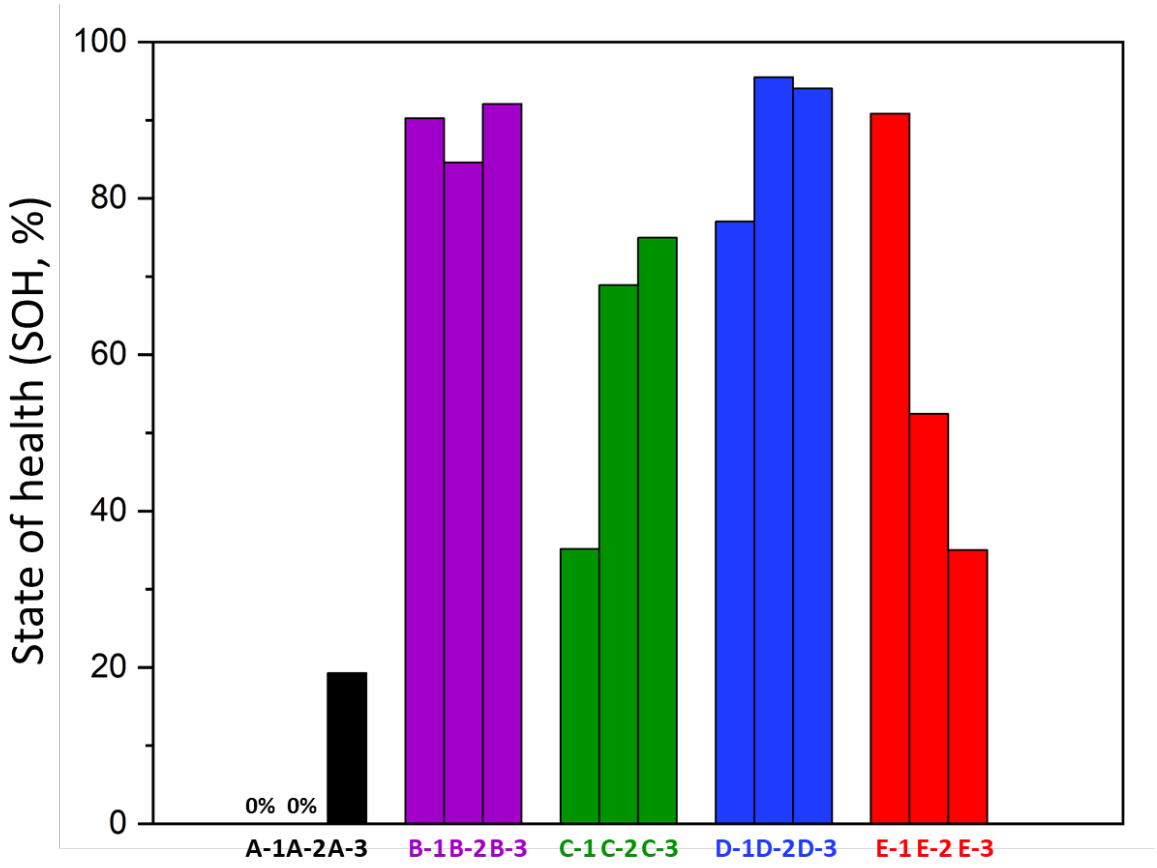

Figure S11. SOH of of 15 batteries from 5 groups.

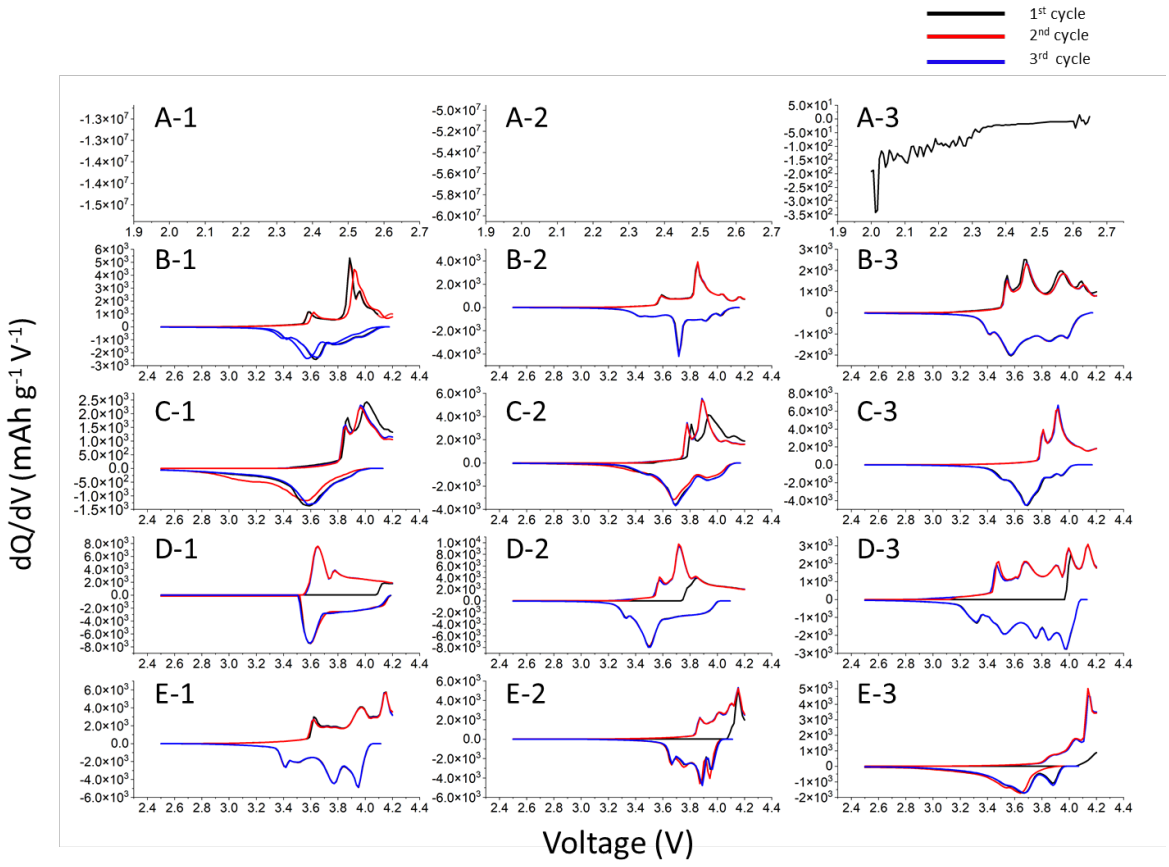

Figure S12. dQ/dV curves of 15 batteries from 5 groups

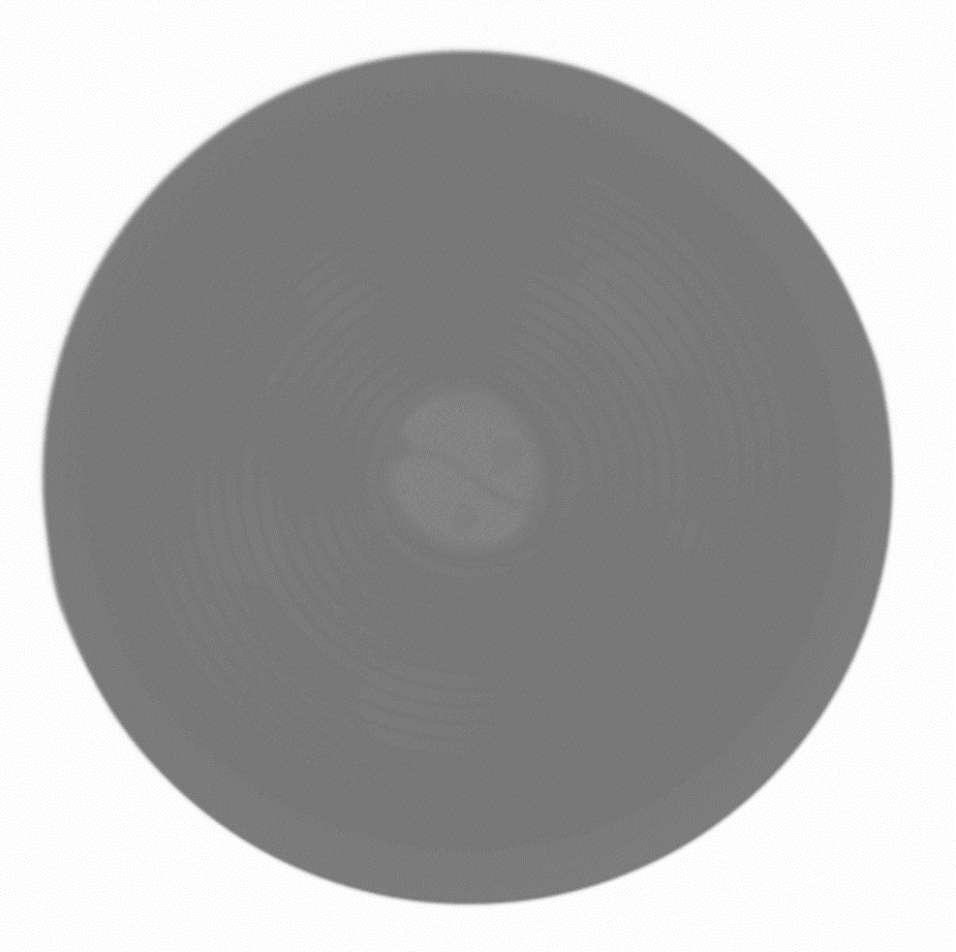

Figure S13. XRT image of Figure 1c, increased by 50% contrast and 30% brightness.