Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Self-assembly of an amino acid derivative as anode interface layer for advanced alkaline Al-air batteries

Lei Guo*[a,b,c], Lei Zhu[a,c], Yue Huang[d], Yan Tan[a,c], Alessandra Gilda Ritacca[e,f], Xingwen Zheng[g], Senlin Leng[a,c] and Baoguo Wang[b]

[a] *School of Material and Chemical Engineering, Tongren University, Tongren 554300, China*
E-mail: chygl@gztrc.edu.cn
[b] *Department of Chemical Engineering, Tsinghua University, Beijing 100084, China*
[c] *Guizhou Provincial Key Laboratory for Cathode Materials of New Energy Battery, Tongren 554300, China*
[d] *College of Materials and Metallurgy, Guizhou University, Guiyang 550025, China*
[e] *Department of Life and Environmental Sciences, Polytechnic University of Marche, Via Brecce Bianche, 60131, Ancona, Italy*
[f] *Center for Synaptic Neuroscience and Technology, Istituto Italiano di Tecnologia, 16132 Genova, Italy*
[g] *Key Laboratory of Material Corrosion and Protection of Sichuan Province, Sichuan University of Science and Engineering, Zigong 643000, China*

Supplementary Figures

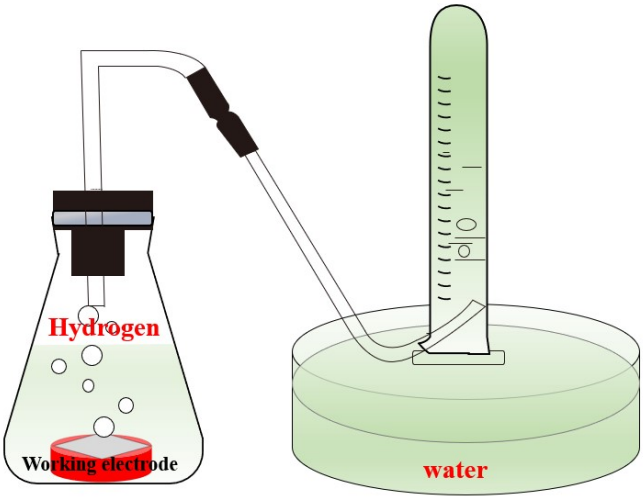

Fig. S1 Diagram of hydrogen collection device by drainage method.

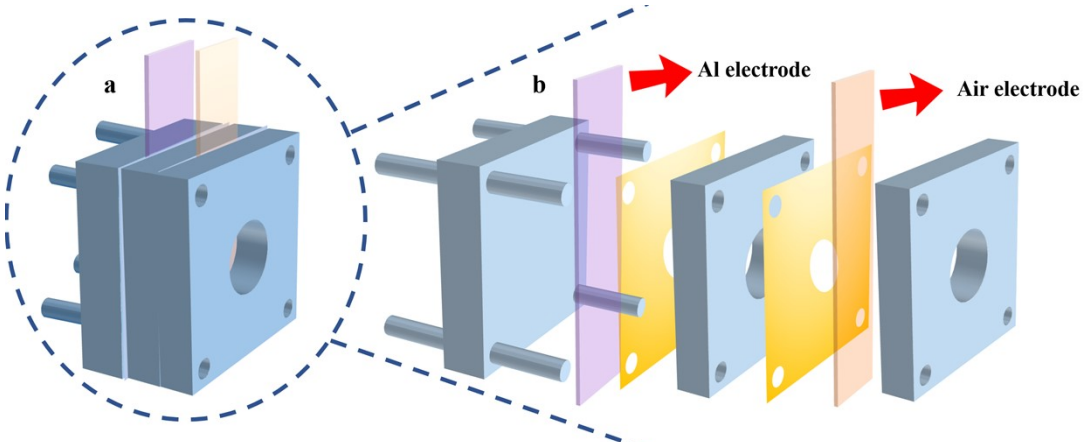

Fig. S2 Diagrams of (a) an integrated Al-air battery device and (b) dismantled components.

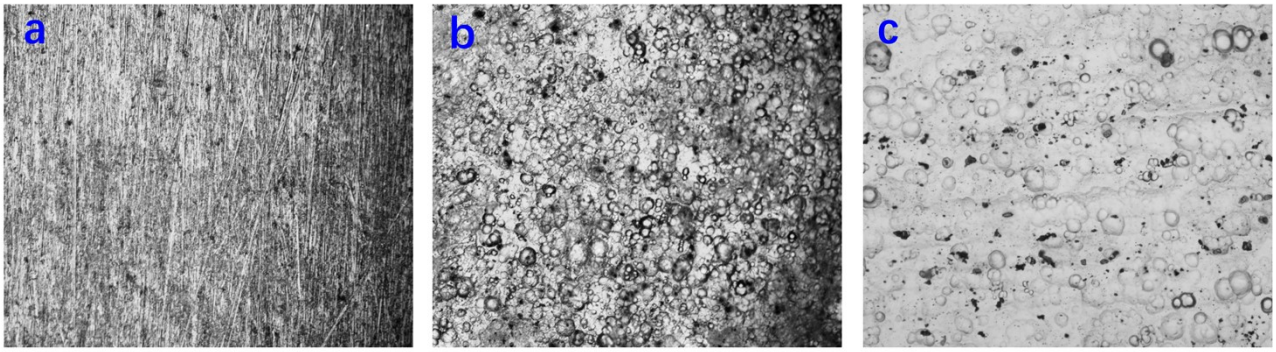

Fig. S3 Metallographic microscope images of Al under different treating conditions: (a) as-polished, (b) blank, (c) 4 M NaOH + 1.5 mM NBLT.

Quantum Chemical Calculations

The adsorption energy of adsorbate molecule on the metal slab, namely E_{ads}, was calculate by the following formula:[1]

$$E_{ads} = E_{mol/slab} - (E_{mol} + E_{slab}) \quad (1)$$

where $E_{mol/slab}$ is the total energies of adsorbate molecules on slab model, E_{inh} is the total energy of isolated adsorbate molecule, E_{slab} is the total energy of the metal slab.

The charge density difference ($\Delta\rho$) is determined by the electron densities of the whole adsorption system ($\rho_{mol/surf}(r)$), the isolated adsorbate molecules ($\rho_{mol}(r)$) and the clean Al(111) surface ($\rho_{surf}(r)$):[2]

$$\Delta\rho = \rho_{mol/surf}(r) - \rho_{mol}(r) - \rho_{surf}(r) \quad (2)$$

References

1 C. Gattinoni and A. Michaelides, *Faraday Discuss.*, 2015, **180**, 439-458.

2 S. B. Liu, *Acta Phys. Chim. Sin.*, 2009, **25**, 590-600.