# Electronic Supplementary Information

## Electrocatalytic Properties of Iron Chalcogenides as Low-Cost Counter Electrode Materials for Dye-sensitized Solar Cells

Jiahao Guo,[a,b] Suxia Liang,[a] Yantao Shi,[a*] Ce Hao,[a] Xuchun Wang[b] and Tingli Ma[a,c*]

[a] State Key laboratory of Fine Chemicals, School of Chemistry, Dalian University of Technology, Dalian, 116024, P. R. China.

E-mail: tinglima@dlut.edu.cn; shiyantao@dlut.edu.cn

[b]College of Chemistry and Materials Engineering, Anhui Science and Technology University, Fengyang, Anhui, 233100, P. R. China.

[c]School Petroleum and Chemical Engineering, Dalian University of Technology, Panjin Campus, Panjin 124221, P. R. China

[d]Graduate School of Life Science and Systems Engineering Kyushu Institute of Technology, Kitakyushu, Fukuoka, 808-0196, Japan

**Table S1** The theoretical lattice constants in comparison with the experimental data.

| | $FeS_2$ | | $FeSe_2$ | | $FeTe_2$ | |
|---|---|---|---|---|---|---|
| | PAW_PBE | Exp. | PAW_PBE | Exp. | PAW_PBE | Exp. |
| *a*(Å) | 5.402 | 5.419 | 4.804 | 4.800 | 5.258 | 5.290 |
| *b*(Å) | 5.402 | 5.419 | 5.780 | 5.776 | 6.250 | 6.270 |
| *c*(Å) | 5.402 | 5.419 | 3.600 | 3.585 | 3.891 | 3.860 |
| V($Å^3$) | 157.6 | 159.1 | 100.0 | 99.4 | 127.2 | 128.0 |

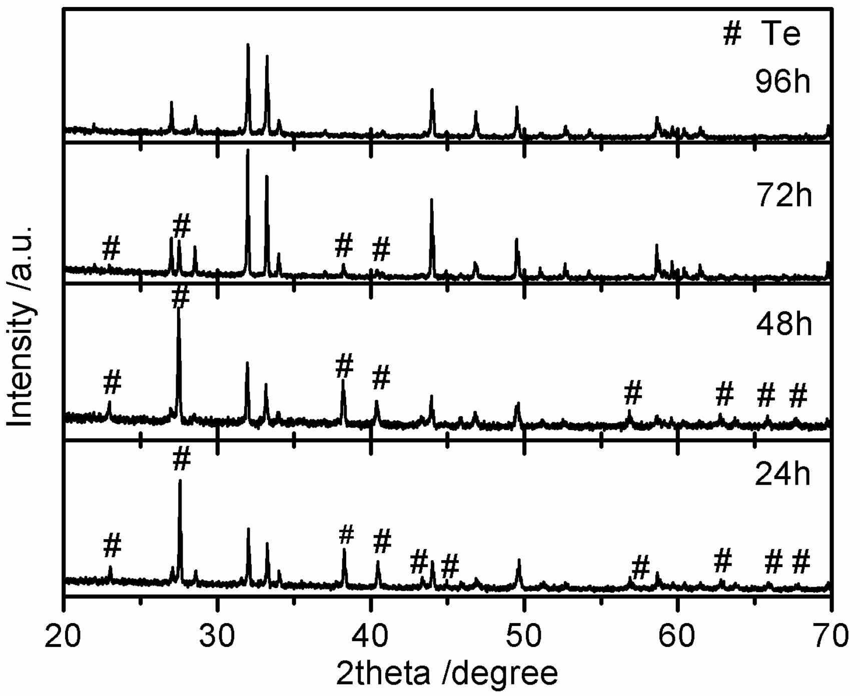

**Figure S1** XRD patterns of the synthesized $FeTe_2$ with different reaction times.

From Fig. S1, the diffraction peaks of the react system were mainly belongs to Te after 24h. Furthermore, the diffraction peaks of $FeTe_2$ was appeared, indicated the formation of $FeTe_2$. With the extension of reaction time, the characteristic diffraction peak intensity of Te decreased gradually while the diffraction peak of $FeTe_2$ gradually increased, predicated that Te gradually transformed into $FeTe_2$. After 96h reaction, XRD pattern displays that only the diffraction peaks of $FeTe_2$ exists in product, indicating that Te has completely transformed to $FeTe_2$, without any impurity peaks in the product.

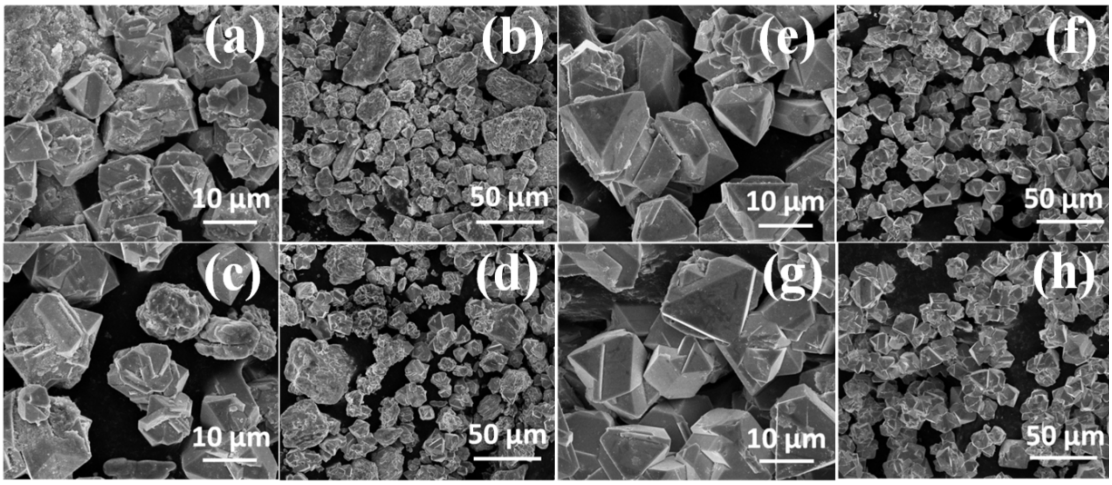

**Figure S2** High- and Low-magnification SEM images of the synthesized $FeTe_2$ with different reaction times. 24h (a, b), 48h (c, d), 72h (e, f), 96h (g, h).

Reactant is composed by some micron particle with irregular morphology. After the reaction starts, some micron particles with a polyhedral shape appear, as shown in Figure 2a and 2b. As the reaction time prolonged, the reactant particles with large grain size were gradually changed into the $FeTe_2$ polyhedron with relatively small size, as shown in Figure 2c and 2d. When the reaction was carried out 72 hours, the reactant has transformed into $FeTe_2$ mostly. The system morphology was mainly polyhedron micron particles. When the reaction time was 96h, reactants have completely transformed to $FeTe_2$, and all product particles change into a relatively regular, uniform polyhedron shape.

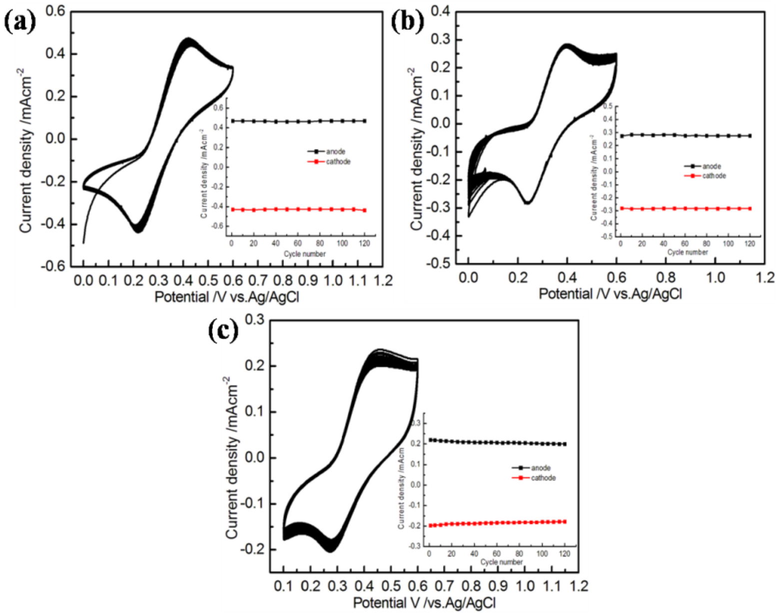

**Figure S3** 120 consecutive CVs of (a) $FeS_2$, (b) $FeSe_2$, (c) $FeTe_2$-based CE in electrolyte solution containing 0.1 M $LiClO_4$, 10 mM LiI, and 1 mM $I_2$ at a scan rate of 10 mV $s^{-1}$; the inset is anodic and cathodic peak current densities versus cycle time.

The electrochemical stability of a CE is of great significance in terms of further application in DSCs. In this work, by means of consecutive CV measurements, we elucidated the electrochemical stability of three iron chalcogenides CEs in electrolyte solution and the result is shown in Figure S3. As can be seen in Figure S3, 120 CV curves coincide very well for three iron chalcogenides. Only slight variation were observed for the current density, indicating that iron chalcogenides-based CEs have good stabilities under practical working conditions.