Energy & Environmental Science

PAPER

Supporting Information

Electrochemical surface charge-inversion from semi-insulating Sb_2Se_3 photoanodes and abrupt photocurrent generation for water splitting

Young Been Kim,[a] Joo Sung Kim,[a] Seung Ki Baek,[a] Young Dae Yun,[a] Sung Woon Cho,[a] Sung Hyeon Jung[a] and Hyung Koun Cho *[a]

[a]School of Advanced Materials Science and Engineering, Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu, Suwon, Gyeonggi-do 16419, Republic of Korea

E-mail: chohk@skku.edu (H. K. Cho).

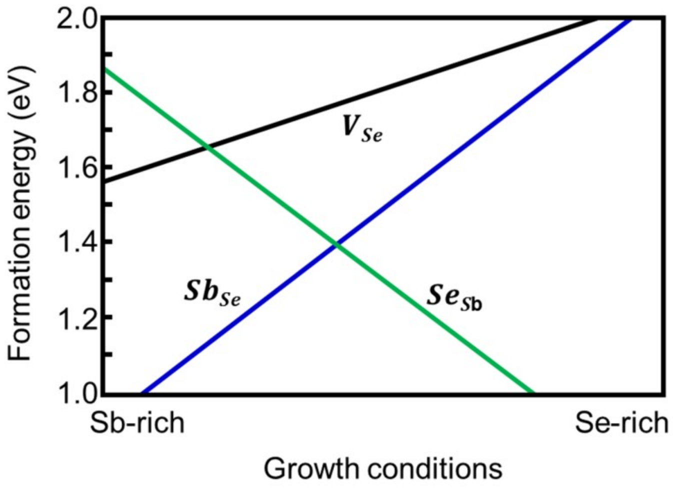

Fig. S1 Formation energy for different defects in the Sb_2Se_3 compounds, where V_{Se} is selenium vacancy defect and Sb_{Se} and Se_{Sb} are the substitutional defects.[10]

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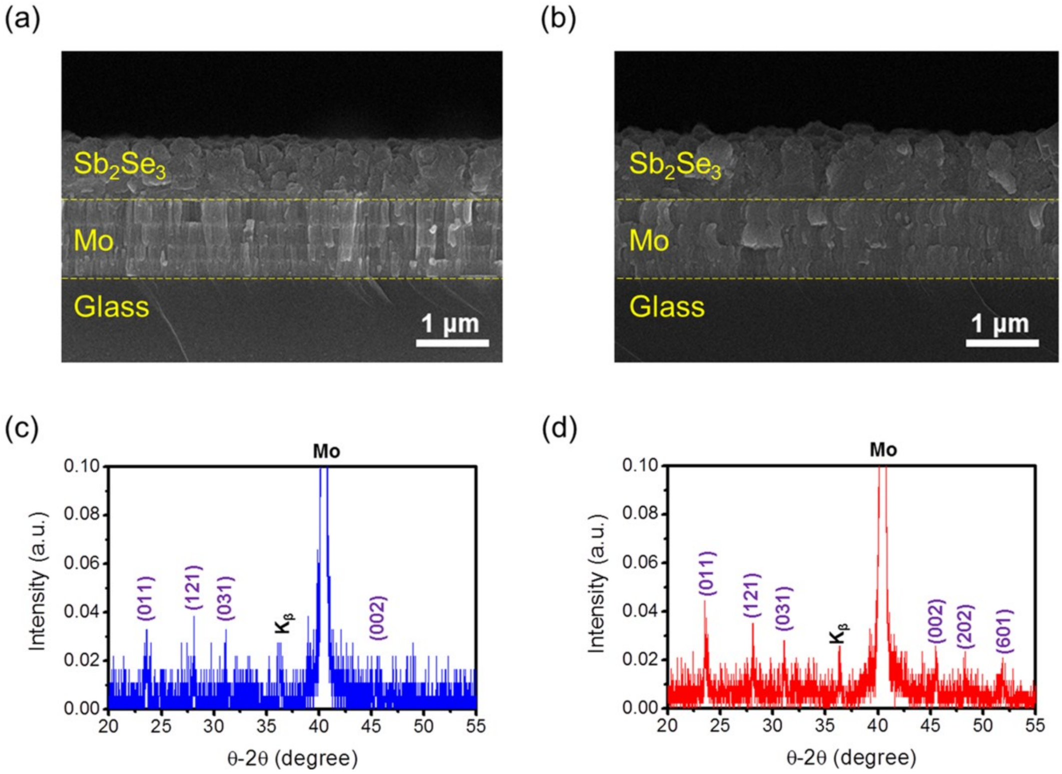

Fig. S2 Cross-sectional SEM images of the Sb_2Se_3 films fabricated at (a) Se-rich for *n*-type and (b) Se-poor for *p*-type. The XRD patterns of (c) the *n*-type and (d) the *p*-type Sb_2Se_3 films.

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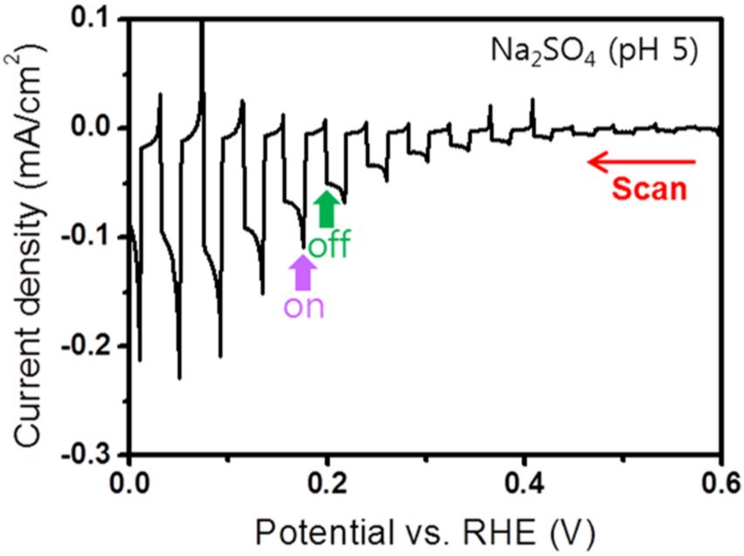

Fig. S3 Linear sweep voltammetry (LSV) result for the *p*-type Sb_2Se_3 measured in 1-M Na_2SO_4 electrolyte buffered with H_2SO_4 (pH 5) under chopped AM 1.5 light illumination.

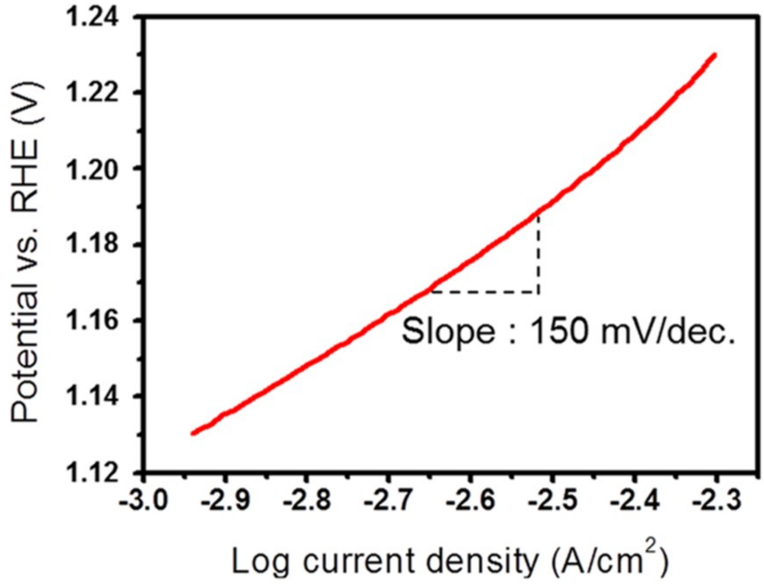

Fig. S4 Tafel plot of the LSV results under illumination at the potential range of the second photocurrent region.

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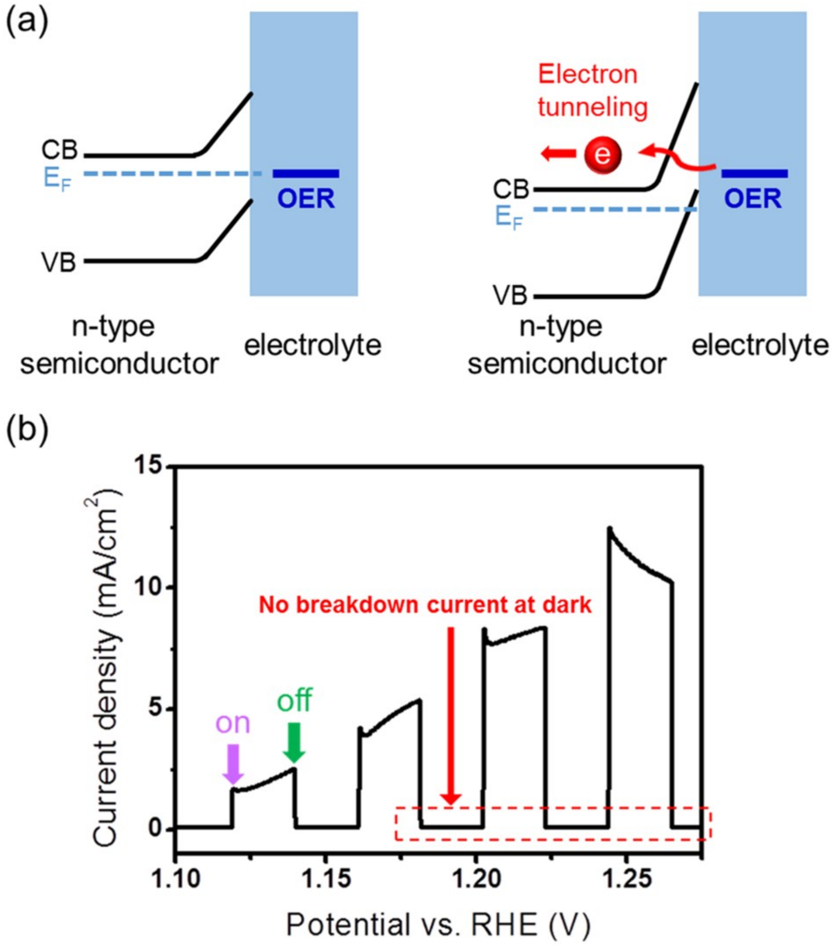

Fig. S5 (a) Energy band diagrams for the *n*-type semiconductor/electrolyte junction (left side) and the breakdown phenomenon via electron tunneling in the reverse bias (right side). (b) Linear sweep voltammetry (LSV) results for Sb_2Se_3 at the potential range above 1.23 V vs. RHE measured in 1-M Na_2SO_4 electrolyte buffered with H_2SO_4 (pH 5) under chopped AM 1.5 light illumination.

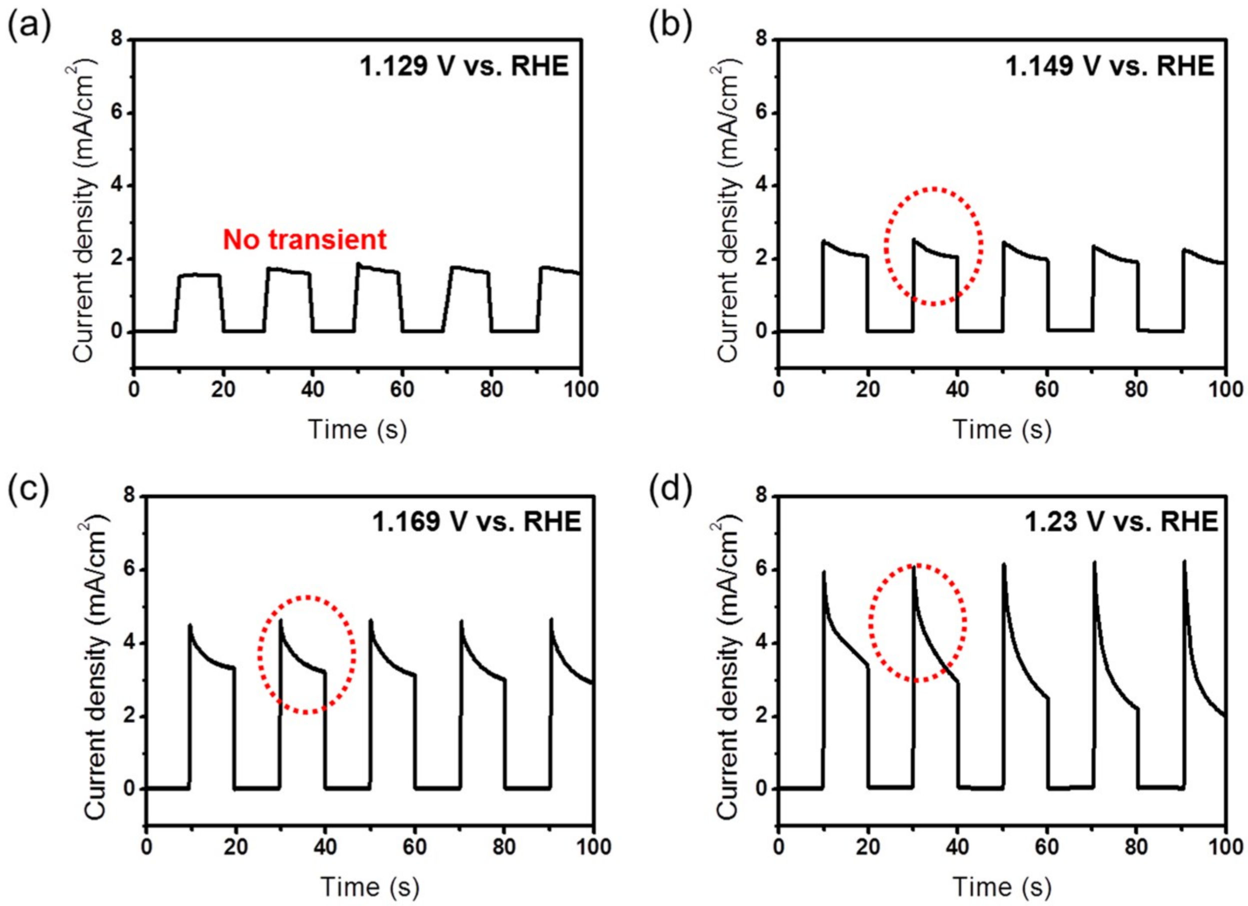

Fig. S6 Chronoamperometry results for *n*-type Sb_2Se_3 under AM 1.5 light chopping in 1-M Na_2SO_4 electrolytes buffered with H_2SO_4 (pH 5) at various potentials vs. RHE: (a) no transient spike of photocurrent at 1.129 V vs. RHE corresponding to the weak inversion state of Sb_2Se_3; (b-d) transient behavior of photocurrent at 1.149 V, 1.169 V, and 1.23 V vs. RHE.