Zinc Selenide Stabilized in a Quadrilateral Network Characterized with Optical Emissions

Kuan-Lin Wang,[†] Cai-Fei Lin,[†] Chin Cheng,^θ Huang, Tzu-Chi,^µ, Lin, Bi-Hsuan,^µ Yu-Lin Xie,[†] Bo-Yuan Wang,[†] Jennifer Kung,[§] Kuang-I Lin,⁸ Kuei-Fang Hsu^{†,*} [†]Department of Chemistry, National Cheng Kung University, Tainan 70101, Taiwan ^θDepartment of Physics, National Cheng Kung University, Tainan 70101, Taiwan ^µNational Synchrotron Radiation Research Center, Hsinchu 300092, Taiwan [§]Department of Earth Science, National Cheng Kung University, Tainan 70101, Taiwan

⁸Core Facility Center, National Cheng Kung University, Tainan 70101, Taiwan

Supplementary Data

Figure S1 The (*hk*0) reflections for (a) the crystal $1 \cdot T$ prepared by quenching at 630 °C and (b) the crystal 1 prepared by slow cooling to 400 °C.

Figure S2 SEM images and EDS spectrum of single crystals for (a) $K_2Zn_{3.03(5)}Se_4$ (1) and (b) $K_2Zn_{2.56(2)}Mg_{0.46(5)}Se_4$ (2).

Figure S3 Observed (black) and calculated (red) powder X-ray diffraction (PXRD) profiles along with the difference plots [Iobs-Icalc] (blue) of the Rietveld refinements for (a) $K_2Zn_3Se_4$ (1) with converged Rwp = 9.59% and GOF = 4.96, and (b) $K_2Mg_{0.5}Zn_{2.5}Se_4$ (2) with converged Rwp = 9.98% and GOF = 3.84.

Figure S4 Differential thermal analysis of the powder samples in two cyclic runs for (a) 1 and (b) 2.

Figure S5 The UV-vis-NIR reflectance spectrum of (a) 1 and (b) 2.

Figure S1 The (*hk*0) reflections for (a) the crystal $1 \cdot T$ prepared by quenching at 630 °C and (b) the crystal **1** prepared by slow cooling to 400 °C.



Figure S2 SEM images and EDS spectrum of single crystals for (a) $K_2Zn_3Se_4$ (1) and (b) $K_2Mg_{0.5}Zn_{2.5}Se_4$ (2).



Figure S3 Observed (black) and calculated (red) powder X-ray diffraction (PXRD) profiles along with the difference plots [Iobs-Icalc] (blue) of the Rietveld refinements for (a) $K_2Zn_{3(5)}Se_4$ (1) with converged Rwp = 9.59% and GOF = 4.96, and (b) $K_2Mg_{0.5}Zn_{2.5}Se_4$ (2) with converged Rwp = 9.98% and GOF = 3.84.



(a)

θ (°)



Figure S4 Differential thermal analysis of the powder samples in two cyclic runs for (a) **1** and (b) **2**.



