The Onset of Copper-Ion Mobility and the Electronic Transition in the Kesterite Cu₂ZnGeSe₄

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Supplementary Information



Figure S1 Rietveld refinement for Cu₂ZnGeS₄ using powder neutron diffraction data collected at 450 K ($\chi^2 = 2.990$). Observed (black crosses), refined (red solid lines), difference (blue bottom line) and calculated background (yellow line) profiles. Reflection positions are marked by olive lines.



Figure S2 Rietveld refinement for Cu₂ZnGeS₄ using powder neutron diffraction data collected at 473 K ($\chi^2 = 2.806$). Observed (black crosses), refined (red solid lines), difference (blue bottom line) and calculated background (yellow line) profiles. Reflection positions are marked by olive lines.



Figure S3 Rietveld refinement for Cu₂ZnGeS₄ using powder neutron diffraction data collected at 473 K ($\chi^2 = 2.064$). Observed (black crosses), refined (red solid lines), difference (blue bottom line) and calculated background (yellow line) profiles. Reflection positions are marked by olive lines.