Magnetic behavior of Cu-intercalated MnPSe3

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There has been a growing interest in magnetic van der Waals (vdW) compounds owing to their two-dimensional magnetic properties, making them particularly suited for the developing field of spintronics. One particular family of vdW compounds, transition-metal phosphorous trichalcogenides (MPX3, M = Mn, Ni, Fe, Cu, Co, etc. X = S and Se), has shown a great potential in the field of magnonics. We study the magnetic nature of MnPSe3 by doping Cu into the structure and analyzing its impact on the long-range magnetic order. Powders of Mn1-xCuxPSe3 have been synthesized using high-temperature solid-state method. Phase purity was confirmed using synchrotron powder X-Ray Diffraction (XRD), Pair Distribution Function (PDF), and powder neutron diffraction. From our PDF and XRD analysis, we find that Cu is most favorably found to be intercalated in the vdW gap of MnPSe3, inducing a long-range magnetic order transformation as observed in magnetic susceptibility and powder neutron diffraction data. Herein, we report magnetic susceptibility, PDF, XRD, carrier density, neutron diffraction data, and DFT calculations for Mn1-xCuxPSe3.