Supplementary Information

$KFeCuTe_2$: A new compound to study the removal of interstitial Fe in layered telluride

Fan Sun‡[a], Zhongnan Guo‡[a], Ning Liu[b], Kun Lin,[c] Da Wang,[b] Wenxia Yuan*[a]

[a] *Department of Chemistry, School of Chemistry and Biological Engineering, University of Science and Technology Beijing, Beijing 100083, China.*

E-mail:wxyuanwz@163.com; Fax:+86-010-62333033; Tel:+86-010-62332221

[b] *Research & Development Center for Functional Crystals, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China.*

[c] *Department of Physical Chemistry, State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing 100083, China.*

‡ *Fan Sun and Zhongnan Guo contribute equally to this work.*

Table S1. Structural parameters for $KFeCuTe_2$ by PXRD Rietveld refinement.

Chemical formula	$K_{0.94}FeCuTe_2$		
Space group	*I*4/*mmm*		
a (Å)	4.2148(4)		
c (Å)	14.7286(11)		
V (Å^3)	261.65(4)		
Z	2		
χ^2	8.79		
R_{wp}（%）	7.80		
$d_{Fe(Cu)-Te}$ (Å)	2.6344(8)		
Atom	*x*	*y*	*z*
K	0	0	0
Fe(Cu)	0	0.5	0.25
Te	0	0	0.3573(1)

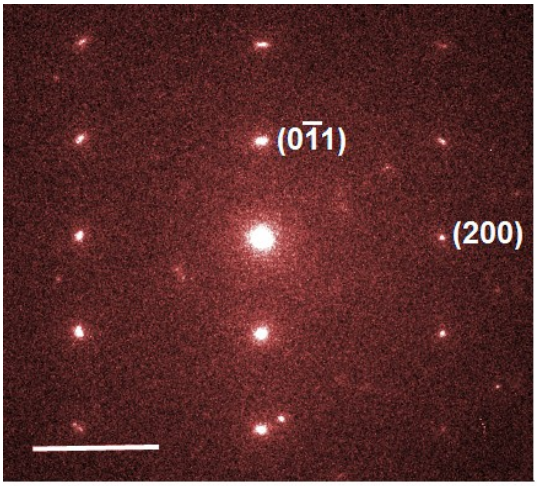

Fig. S1 SAED pattern of $KFeCuTe_2$ crystal along the [011] zone axes, showing the tetragonal unit cell. The scale bar in the left bottom is 5 1/nm.

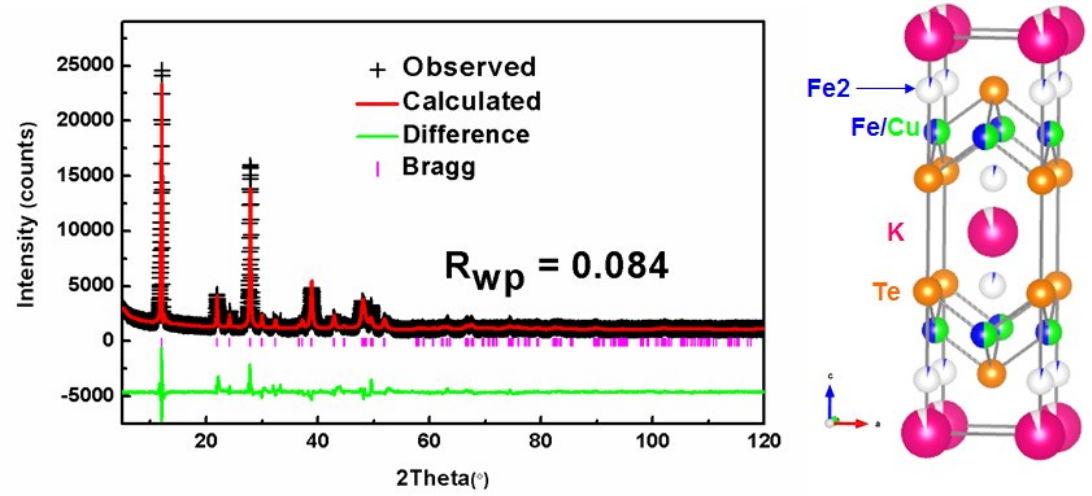

Fig. S2 Rietveld refinement with the structure model containing 4% interstitial Fe atoms (0.5, 0.5, z), resulting the R_{wp} = 0.084, which is larger than that without the interstitial Fe (0.078).

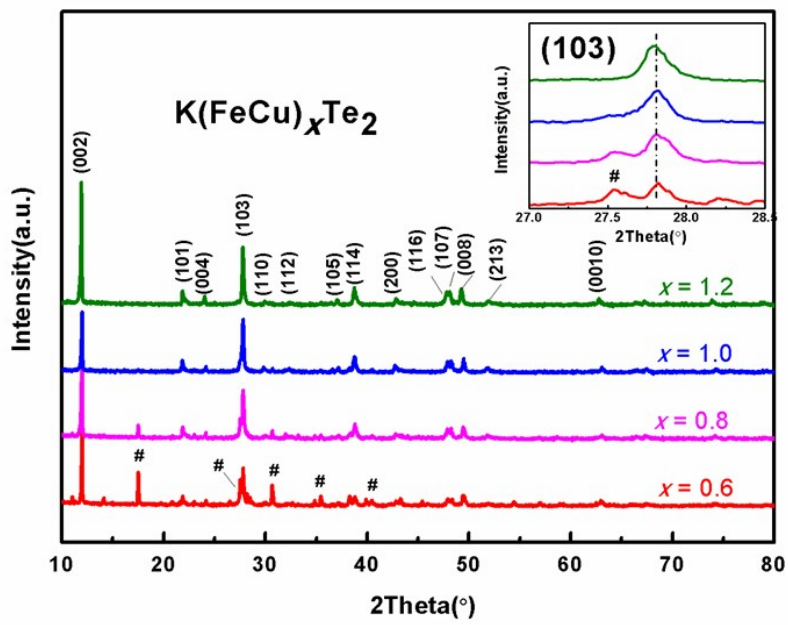

Fig. S3 PXRD patterns of the crystals grown from different nominal compositions. Inset shows the enlarged (103) diffraction peak with the same location, suggesting that the obtained main phases in different patterns are the same. # represents the impurity of K_2Te_3 (ICDD: 71-0490).

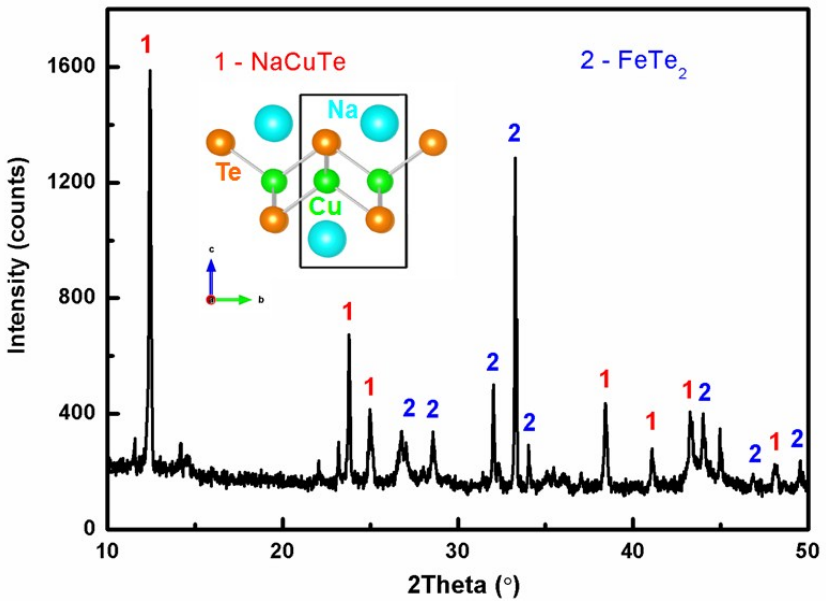

Fig. S4 PXRD pattern of the nominal compostion $NFeCuTe_2$, showing the products of NaCuTe and $FeTe_2$. Inset shows the crystal structure of NaCuTe.

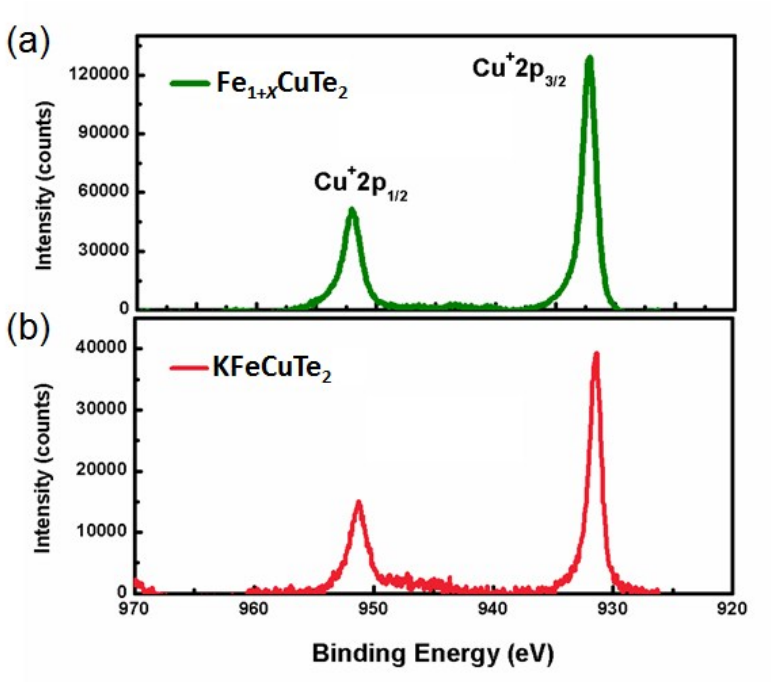

Fig. S5 XPS Cu spectra of (a) $Fe_{1+x}CuTe_2$ and (b) $KFeCuTe_2$, showing +1 valence.[1]

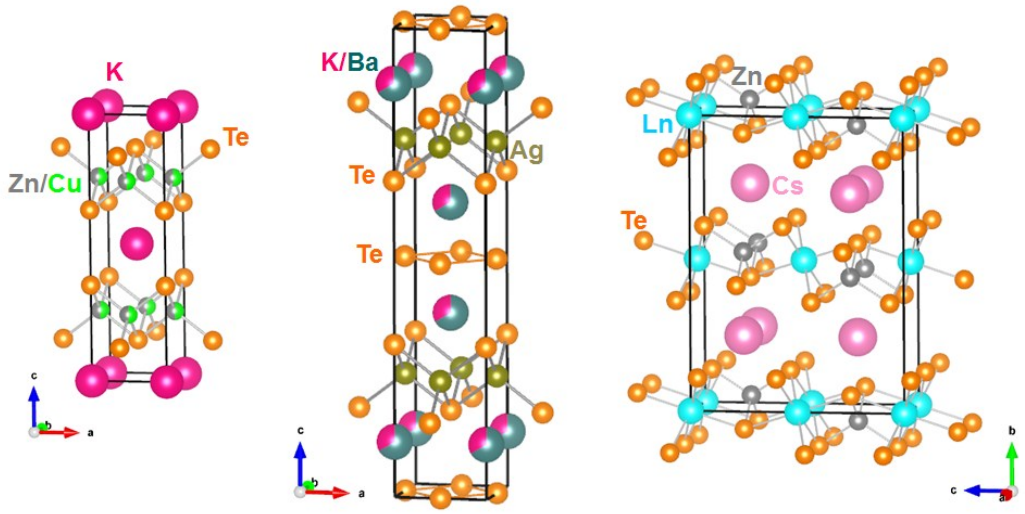

Fig. S6 The crystal structures of some typical layered transition metal tellurides: $KZnCuTe_2$,[2] $K_{0.33}Ba_{0.67}AgTe_2$[3] and Cs*Ln*ZnTe_3 (*Ln*= rare earth)[4].

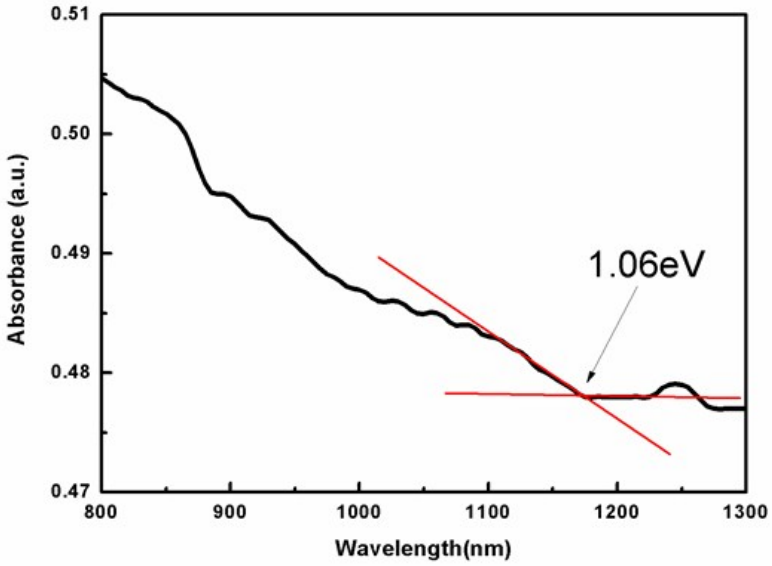

Fig. S7 UV−vis−NIR diffuse-reflectance spectra of $KFeCuTe_2$, showing a band gap E_g = 1.06 eV.

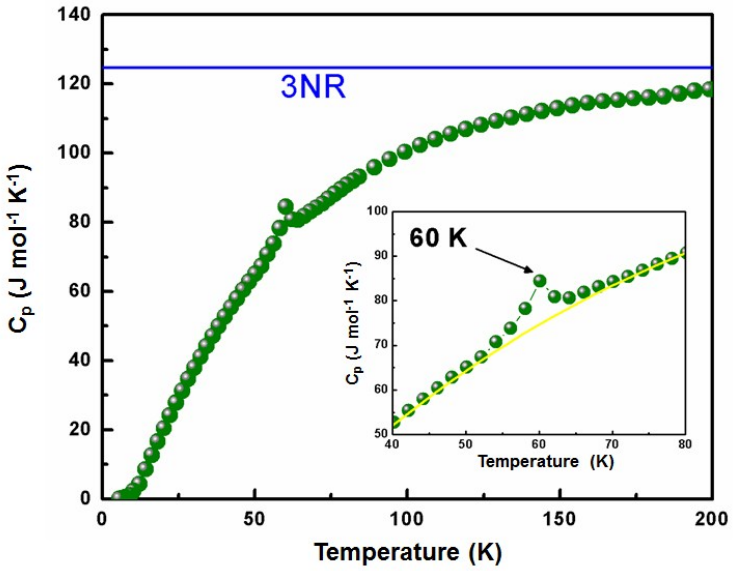

Fig. S8 Temperature dependence of specific heat for $KFeCuTe_2$. The inset shows the enlarged area near the magnetic transition at 60 K, with the yellow solid curve representing the lattice contribution by a polynomial. The blue line is the Dulong-Petit value of 3*NR*, which approaches the high temperature heat capacity.

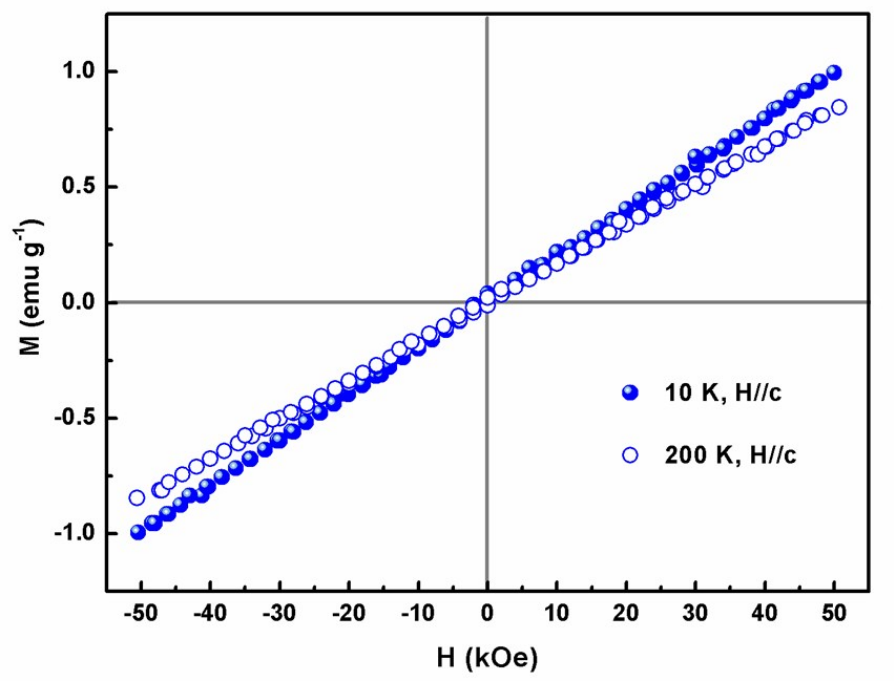

Fig. S9 Magnetization loops M(H) with H//c at 10 K and 200 K.

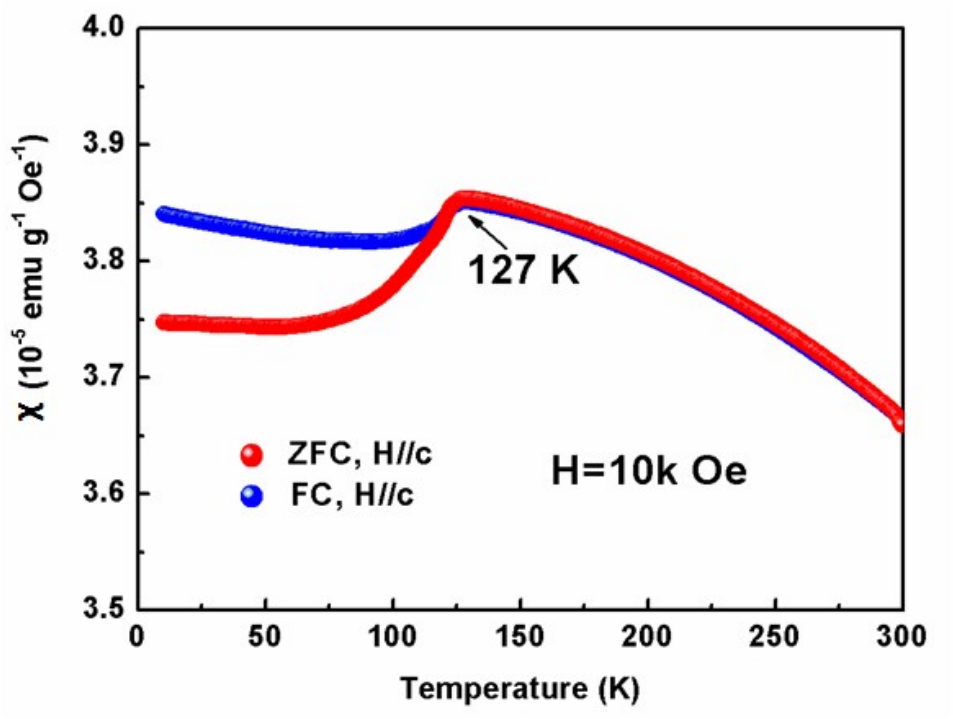

Fig. S10 Temperature dependence of magnetic susceptibility of the sample after air exposure for a few days, showing an anomaly at 127 K and the rising susceptibility of FC curve at low temperature, which is attributed to the formation of Fe_3O_4 impurity.

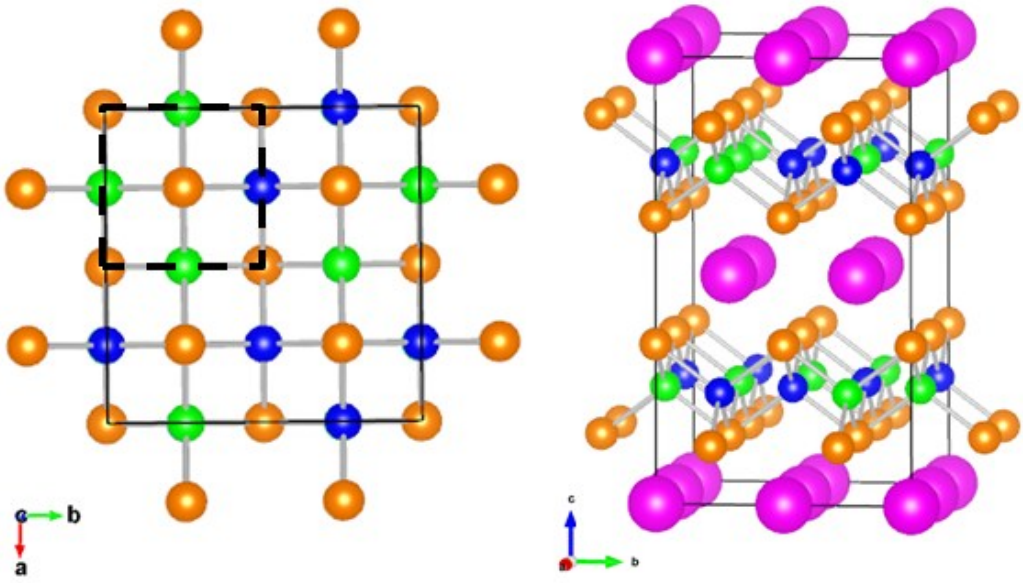

Fig. S11 The structural model used in the first principle calculation: a 2×2 supercell with the randomly distributed Fe/Cu atoms.

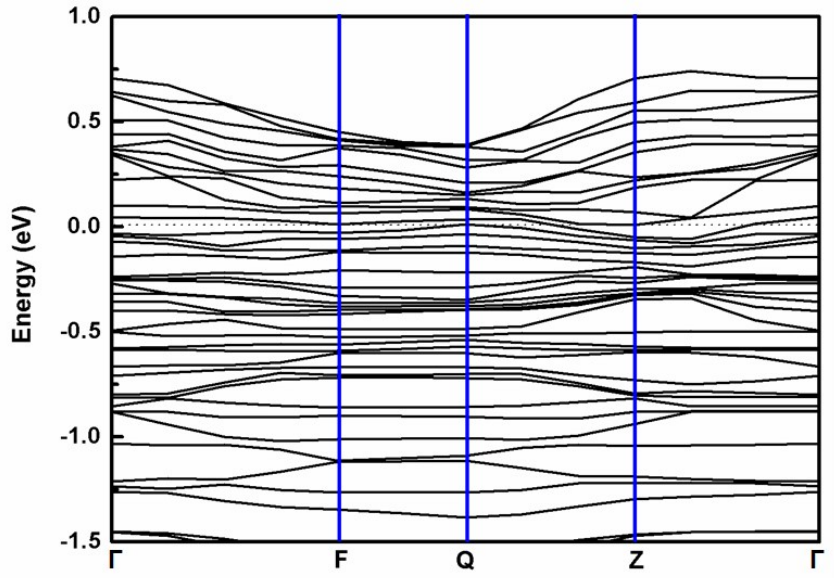

Fig. S12 The band structure of non-magnetic $KFeCuTe_2$, showing a metallic state.

References

1. D. Cahen, P. J. Ireland, L. L. Kazmerski and F. A. Thiel, *Journal of Applied Physics*, 1985, **57**, 4761-4771.

2. J. Li, H.-Y. Guo, R. A. Yglesias and T. J. Emge, *Chemistry of Materials*, 1995, **7**, 599-601.
3. X. Zhang, X. Li, B. Foran, S. Lee, S. Guo, S. Hogan, S. Kannewurf and M. G. Kanatzidis, *Journal of the American Chemical Society*, 1995, **117**, 10513-10520.
4. J. Yao, B. Deng, L. J. Sherry, A. D. McFarland, D. E. Ellis, R. P. Van Duyne and J. A. Ibers, *Inorganic Chemistry*, 2004, **43**, 7735-7740.