Supplemental Materials for

Enhanced thermal and dielectric properties of CaCu₃Ti₄O₁₂ by (Fe,La)-co-doping

Ruifeng Wu[a,b], Haibing Li[c], Yafei Liu[a,b], Aimin Chang[a, *], Bo Zhang[a,*]

[a]*Key Laboratory of Functional Materials and Devices for Special Environments of CAS; Xinjiang Key Laboratory of Electronic Information Materials and Devices; Xinjiang Technical Institute of Physics & Chemistry of CAS, Urumqi, 830011, China*

[b]*Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing, 100049, China*

[c]*Xinjiang Uygur Autonomous Region Research Institute of Measurement and Testing, Urumqi, 830011, China*

*Corresponding author.

E-mail address: changam@ms.xjb.ac.cn (Aimin Chang)

zhangbocas@ms.xjb.ac.cn (Bo Zhang)

Supplementary Tables

Table S1. The structural parameters of $Ca_{1-y}La_yCu_{2.5}Fe_{0.5}Ti_4O_{12}$ samples.

Sample	$CaCu_{2.5}Fe_{0.5}Ti_4O_{12}$	$Ca_{0.9}La_{0.1}Cu_{2.5}Fe_{0.5}Ti_4O_{12}$	$Ca_{0.8}La_{0.2}Cu_{2.5}Fe_{0.5}Ti_4O_{12}$	$Ca_{0.7}La_{0.3}Cu_{2.5}Fe_{0.5}Ti_4O_{12}$
A	$a=b=c, \alpha=\beta=\gamma=90°$			
Space group	Im-3			
Lattice constant (Å)	7.3919(6)	7.3959(10)	7.4028(8)	7.4086(9)
Volume (Å³)	403.89(10)	404.552(17)	405.691(14)	406.638(15)
Density (g/cm³)	5.051	5.043	5.029	5.017
R_{WP} **(%)**	5.82	6.53	6.17	6.7
R_P **(%)**	4.47	5.02	4.59	4.88
χ^2	1.71	2.16	1.87	2.21

Supplementary Figures
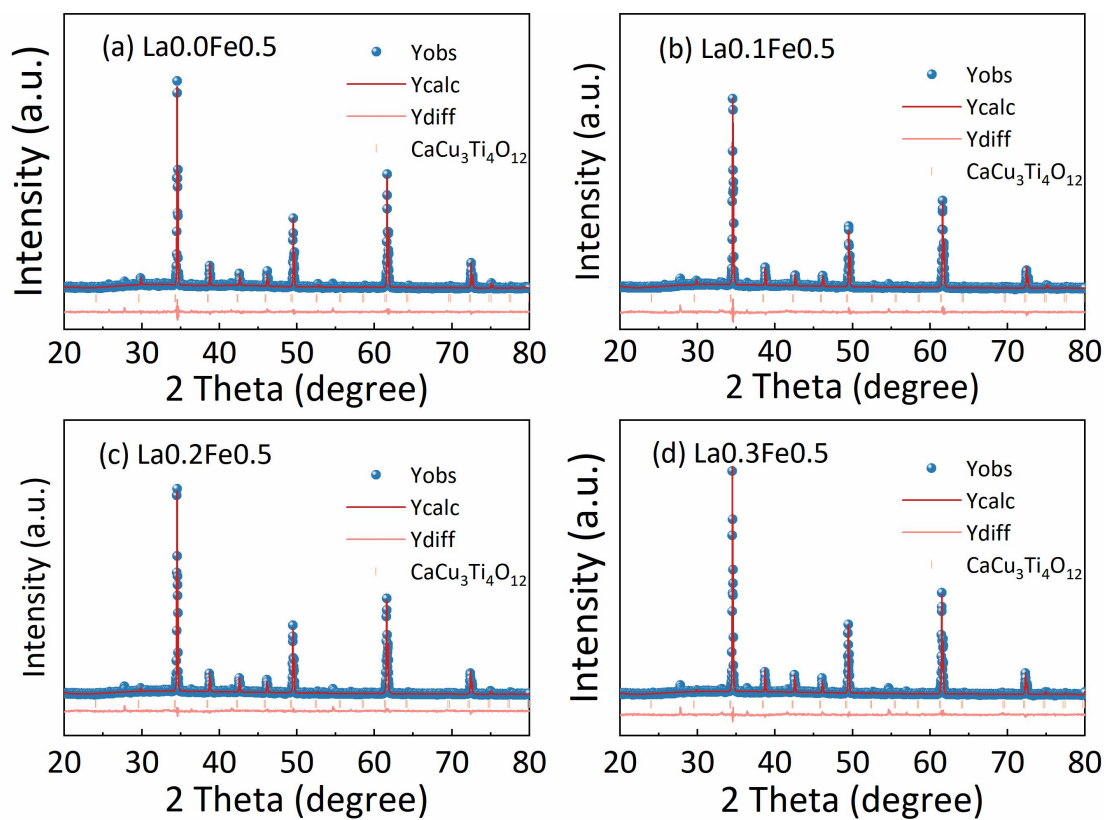
Figure S1. Rietveld refinement results for the $Ca_{1-y}La_yCu_{2.5}Fe_{0.5}Ti_4O_{12}$ samples. (a) La0.0Fe0.5, (b) La0.1Fe0.5, (c) La0.2Fe0.5 and (d) La0.3Fe0.5.
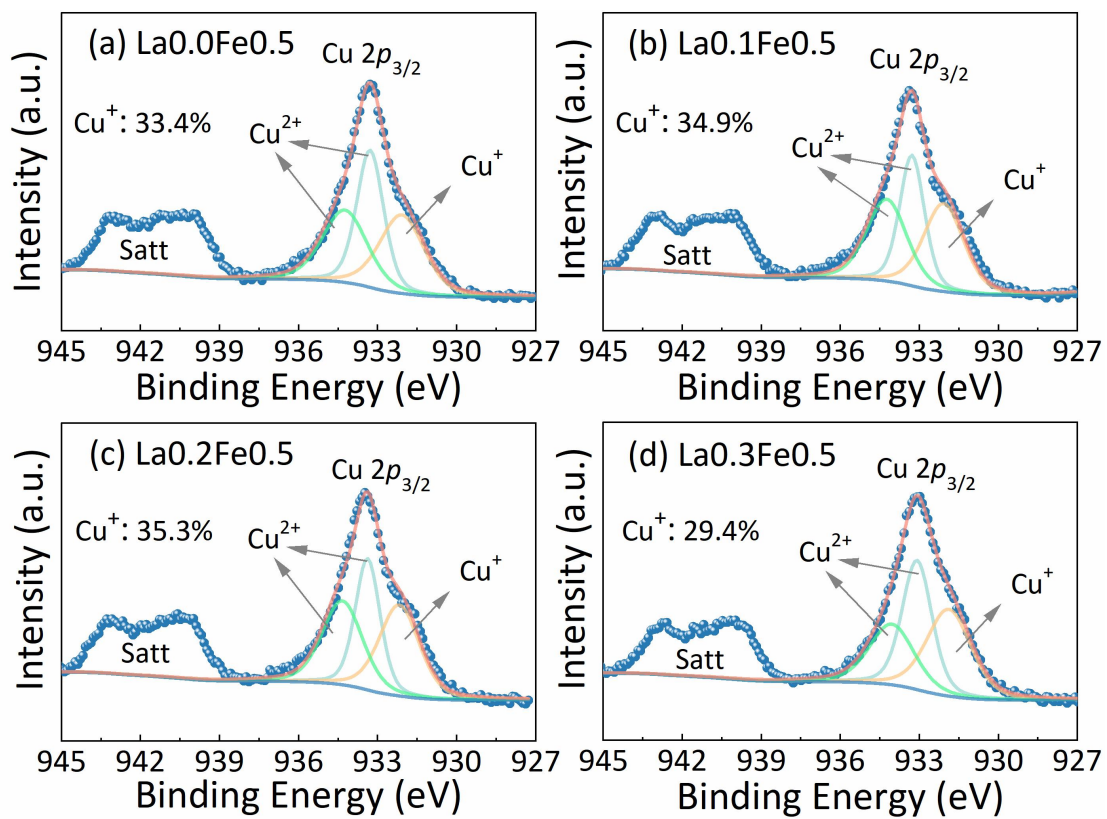
Figure S2. XPS spectrum and fitting curves of Cu $2p$ spectrum for $Ca_{1-y}La_yCu_{2.5}Fe_{0.5}Ti_4O_{12}$ samples. (a) La0.0Fe0.5, (b) La0.1Fe0.5, (c) La0.2Fe0.5 and (d) La0.3Fe0.5.
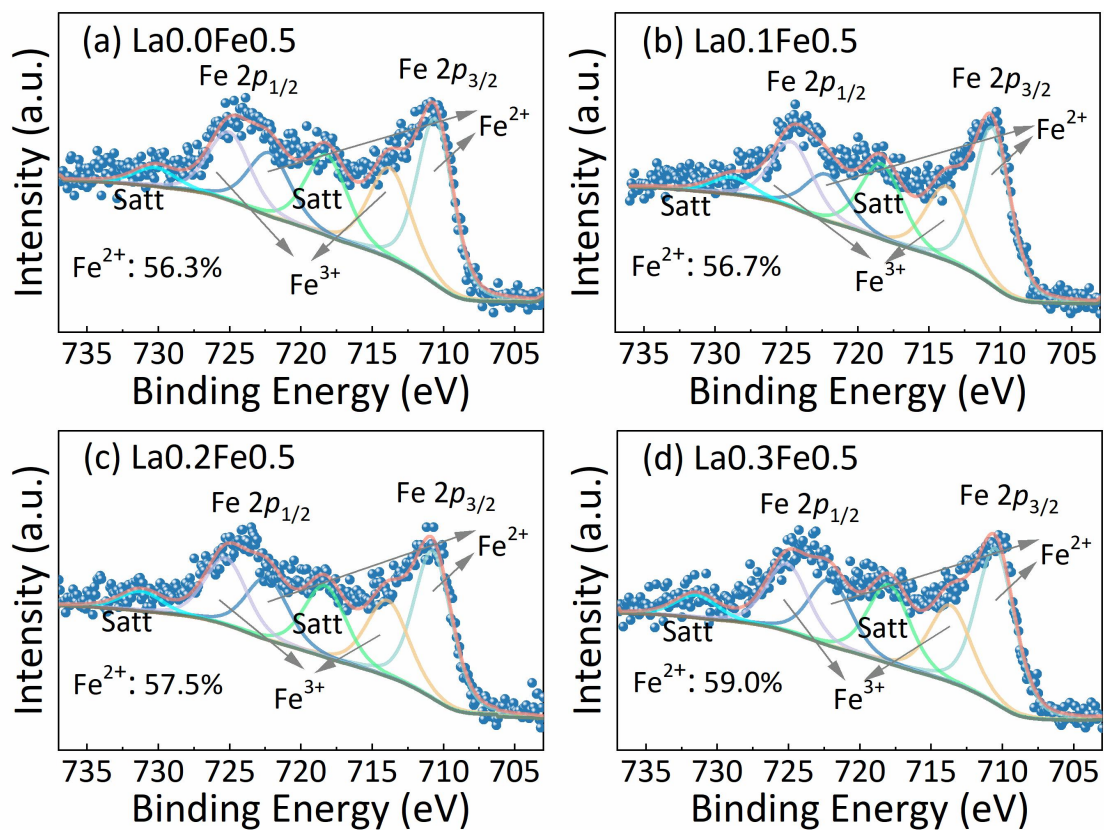
Figure S3. XPS spectrum and fitting curves of Fe $2p$ spectrum for $Ca_{1-y}La_yCu_{2.5}Fe_{0.5}Ti_4O_{12}$ samples. (a) La0.0Fe0.5, (b) La0.1Fe0.5, (c) La0.2Fe0.5 and (d) La0.3Fe0.5.
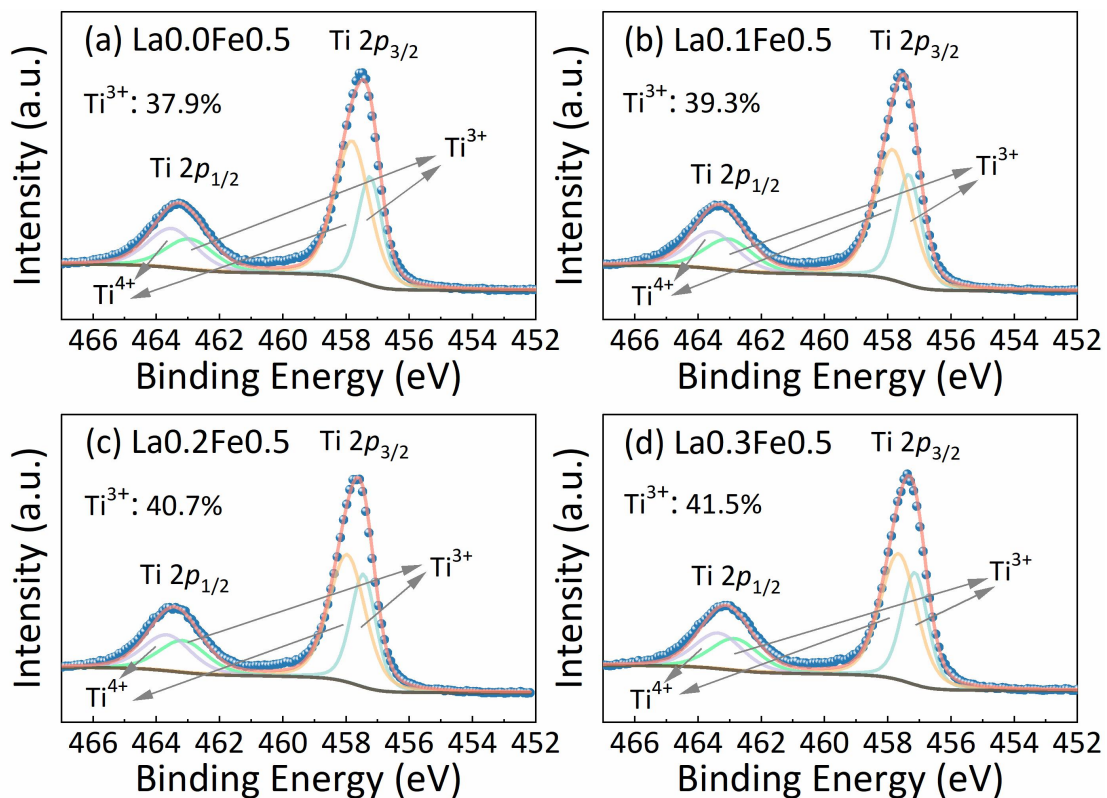
Figure S4. XPS spectrum and fitting curves of Ti $2p$ spectrum for $Ca_{1-y}La_yCu_{2.5}Fe_{0.5}Ti_4O_{12}$ samples. (a) La0.0Fe0.5, (b) La0.1Fe0.5, (c) La0.2Fe0.5 and (d) La0.3Fe0.5.
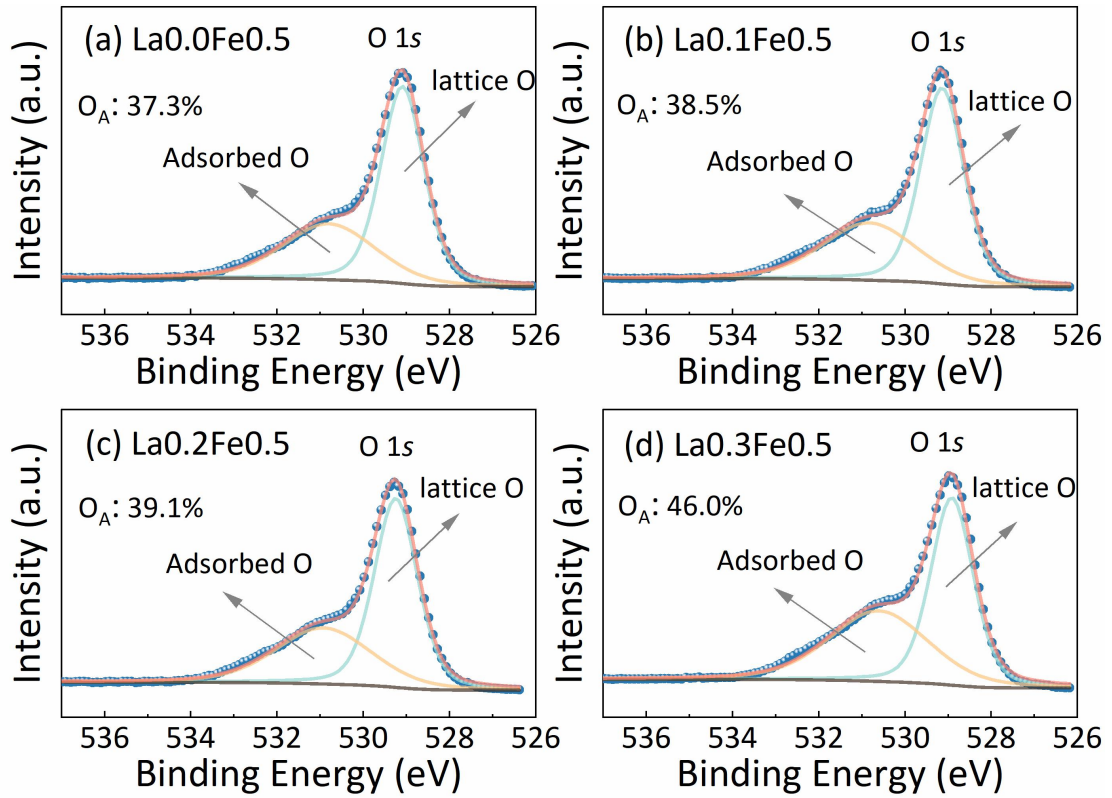
Figure S5. XPS spectrum and fitting curves of O 1s spectrum for $Ca_{1-y}La_yCu_{2.5}$ $Fe_{0.5}Ti_4O_{12}$ samples. (a) La0.0Fe0.5, (b) La0.1Fe0.5, (c) La0.2Fe0.5 and (d) La0.3Fe0.5.
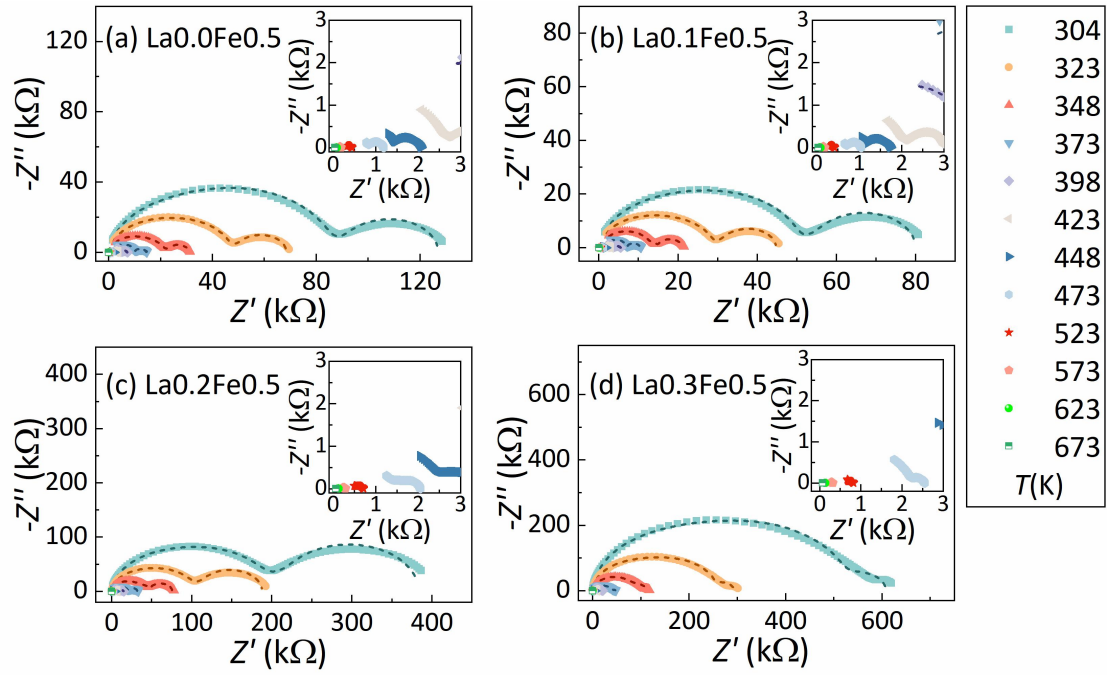
Figure S6. Impedance spectrum of the $Ca_{1-y}La_yCu_{2.5}Fe_{0.5}Ti_4O_{12}$ samples in the different temperature range of 304–673 K. (a) La0.0Fe0.5, (b) La0.1Fe0.5, (c) La0.2Fe0.5 and (d) La0.3Fe0.5.
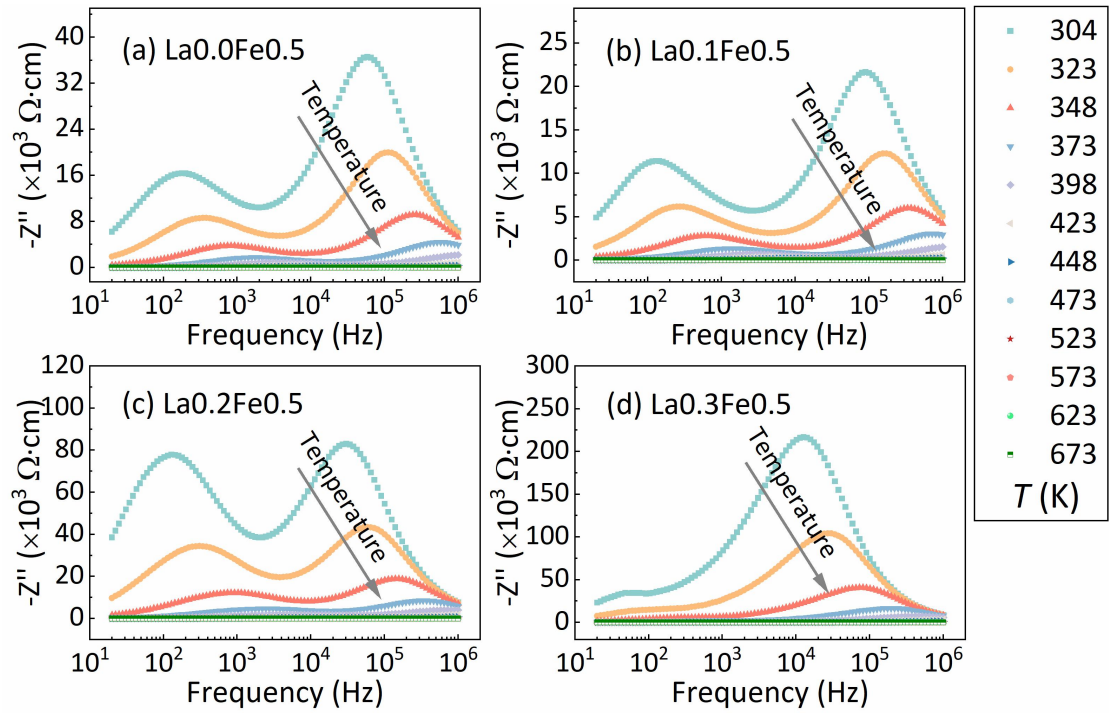
Figure S7. Frequency dependence of Z" for the Ca$_{1-y}$La$_y$Cu$_{2.5}$Fe$_{0.5}$Ti$_4$O$_{12}$ samples. (a) La0.0Fe0.5, (b) La0.1Fe0.5, (c) La0.2Fe0.5 and (d) La0.3Fe0.5.
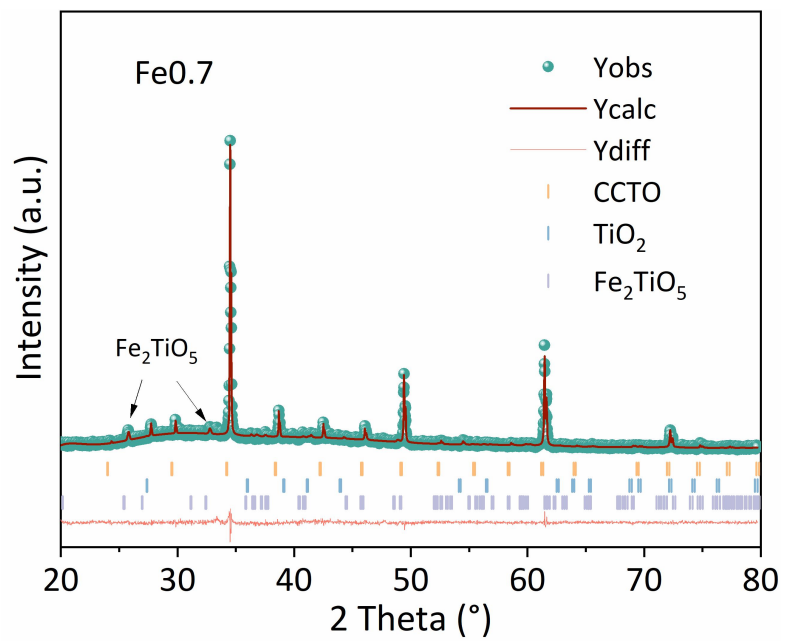
Figure S8. Rietveld refinement results for the CaCu$_{2.3}$Fe$_{0.7}$Ti$_4$O$_{12}$ samples.