Supplementary Information for

Cationic composition engineering in double perovskite $XLaLiTeO_6:Eu^{3+}$ (X = Ba, Sr, Ca, Mg) toward the efficient and thermally stable red luminescence for domestic white-LEDs

Jing Zhu, Tongsheng Yang, Hong Li, Yuefei Xiang, Ruitong Song, Hongzhi Zhang*

Yunnan Key Laboratory of Carbon Neutrality and Green Low-carbon Technologies, Key Laboratory of LCR Materials and Devices of Yunnan Province, School of Materials and Energy, Yunnan University, Kunming 650091, China

*Corresponding author

E-mail: zhanghz@ynu.edu.cn

This supplement contains:

Supplemental Figure S1-S9, Table S1-S3

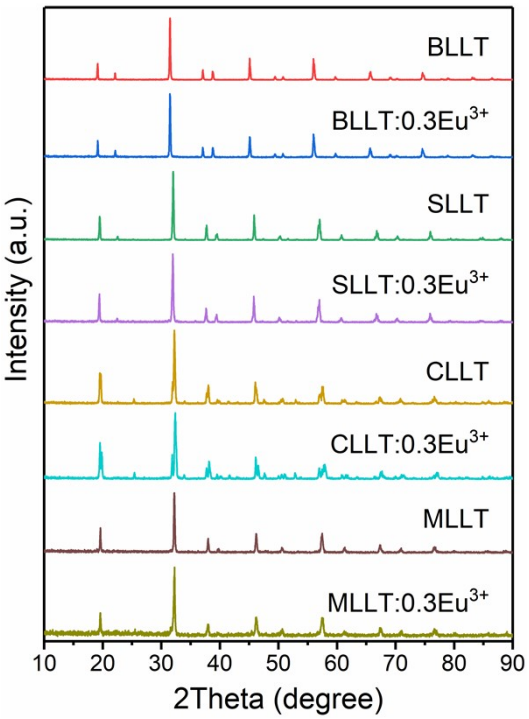

Figure S1. XRD patterns of XLLT(:Eu^{3+}) samples.

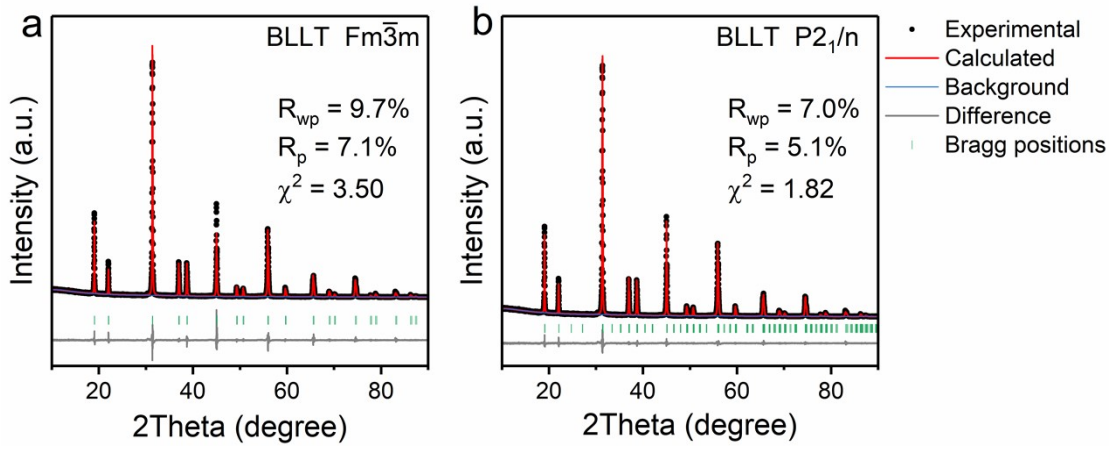

Figure S2. Rietveld refinements of the XRD profile of BLLT host using initial models in space groups (a) $Fm\bar{3}m$ and (b) $P2_1/n$, respectively.

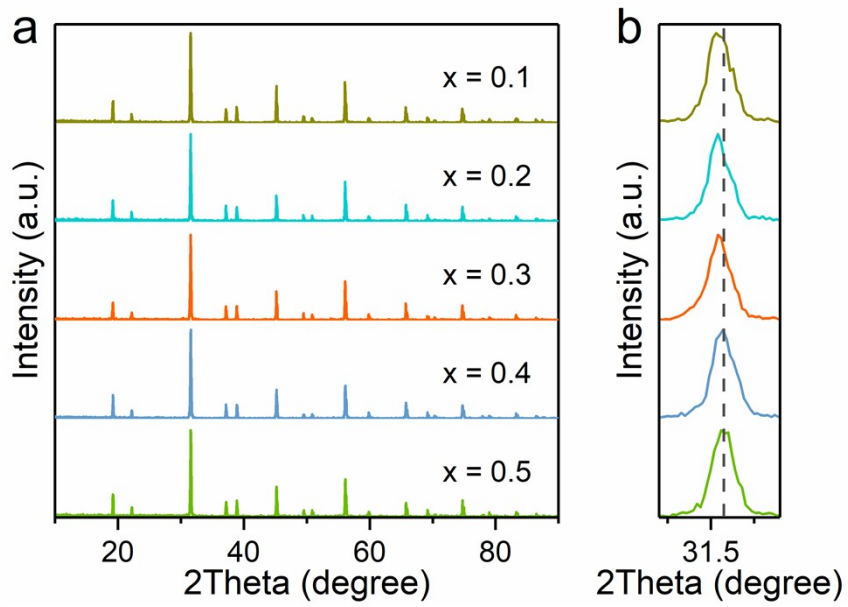

Figure S3. (a) XRD patterns of BLLT:xEu^{3+} samples and (b) the enlarged versions.

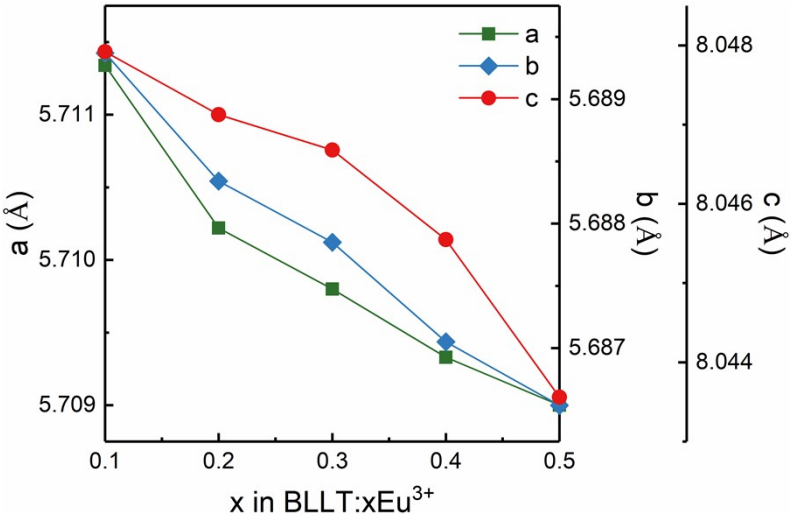

Figure S4. Changes of the cell parameters with x in BLLT:xEu^{3+}.

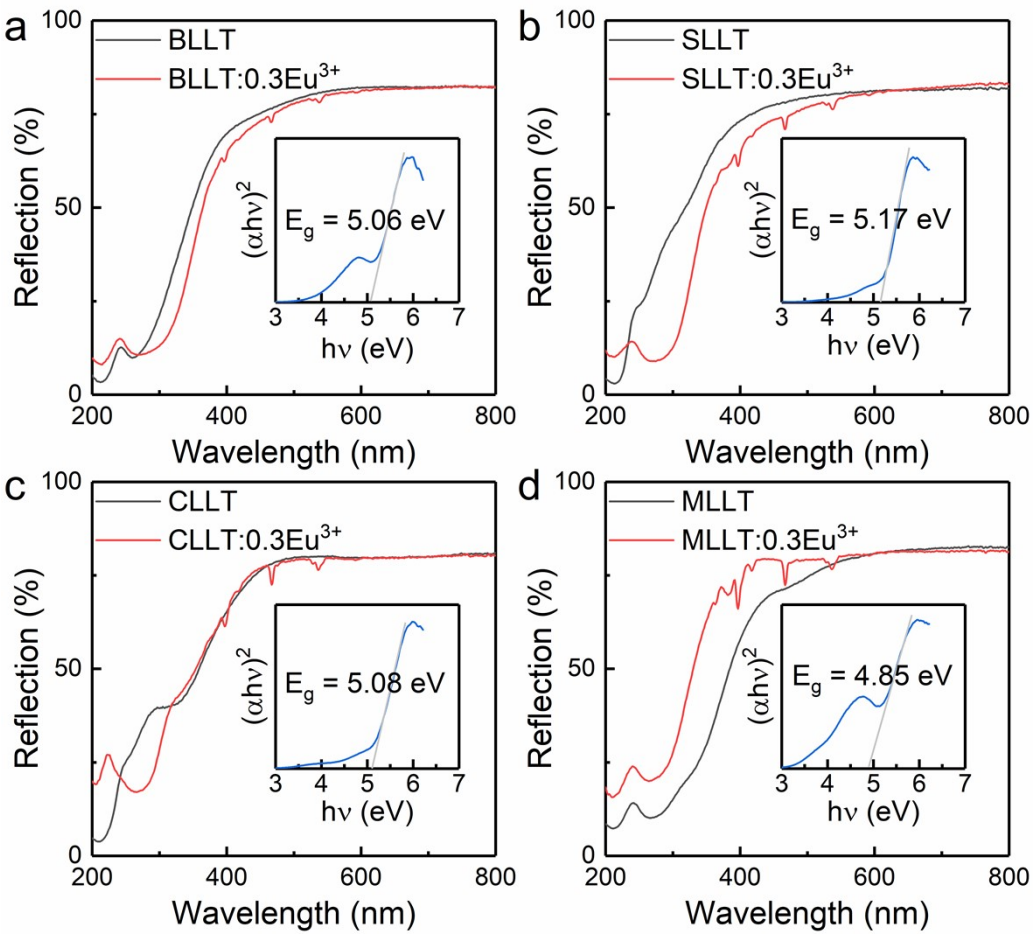

Figure S5. UV-vis diffuse reflectance spectra of (a) BLLT(:Eu^{3+}), (b) SLLT(:Eu^{3+}), (c) CLLT(:Eu^{3+}) and (d) MLLT(:Eu^{3+}). The insets show the Tauc-plots of the hosts.

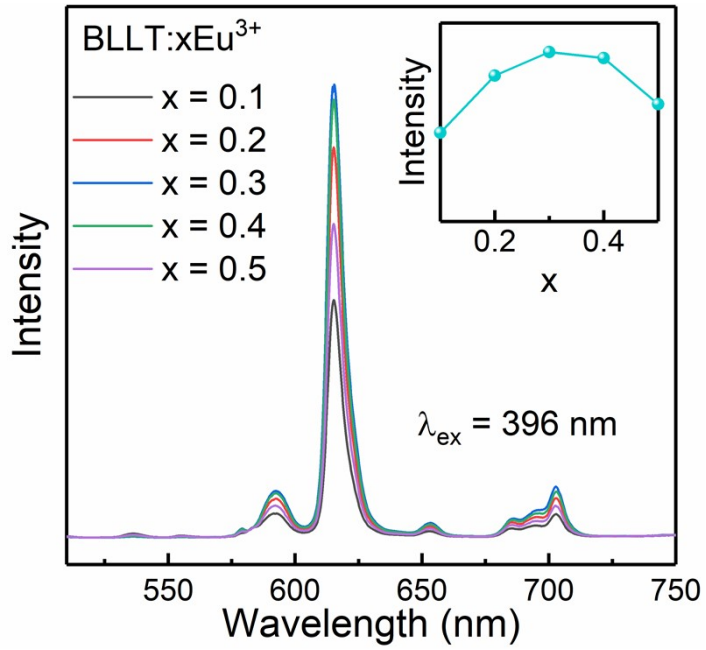

Figure S6. The emission spectra of BLLT:xEu^{3+}, and the inset depicts emission intensity as a function of x.

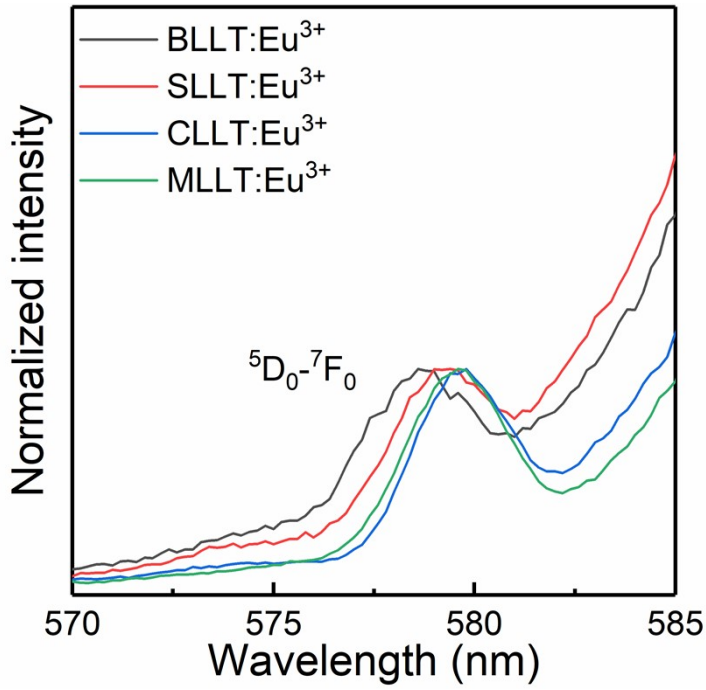

Figure S7. $^5D_0$-$^7F_0$ transition spectra of XLLT:Eu^{3+} (X = Ba, Sr, Ca and Mg).

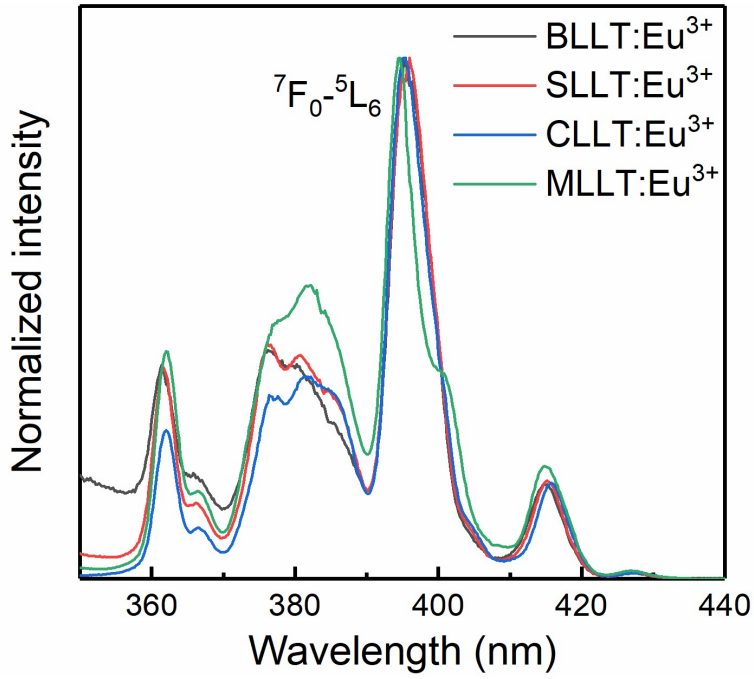

Figure S8. Normalized $^{7}F_{0}$-$^{5}L_{6}$ transition spectra of XLLT:Eu^{3+} (X = Ba, Sr, Ca and Mg).

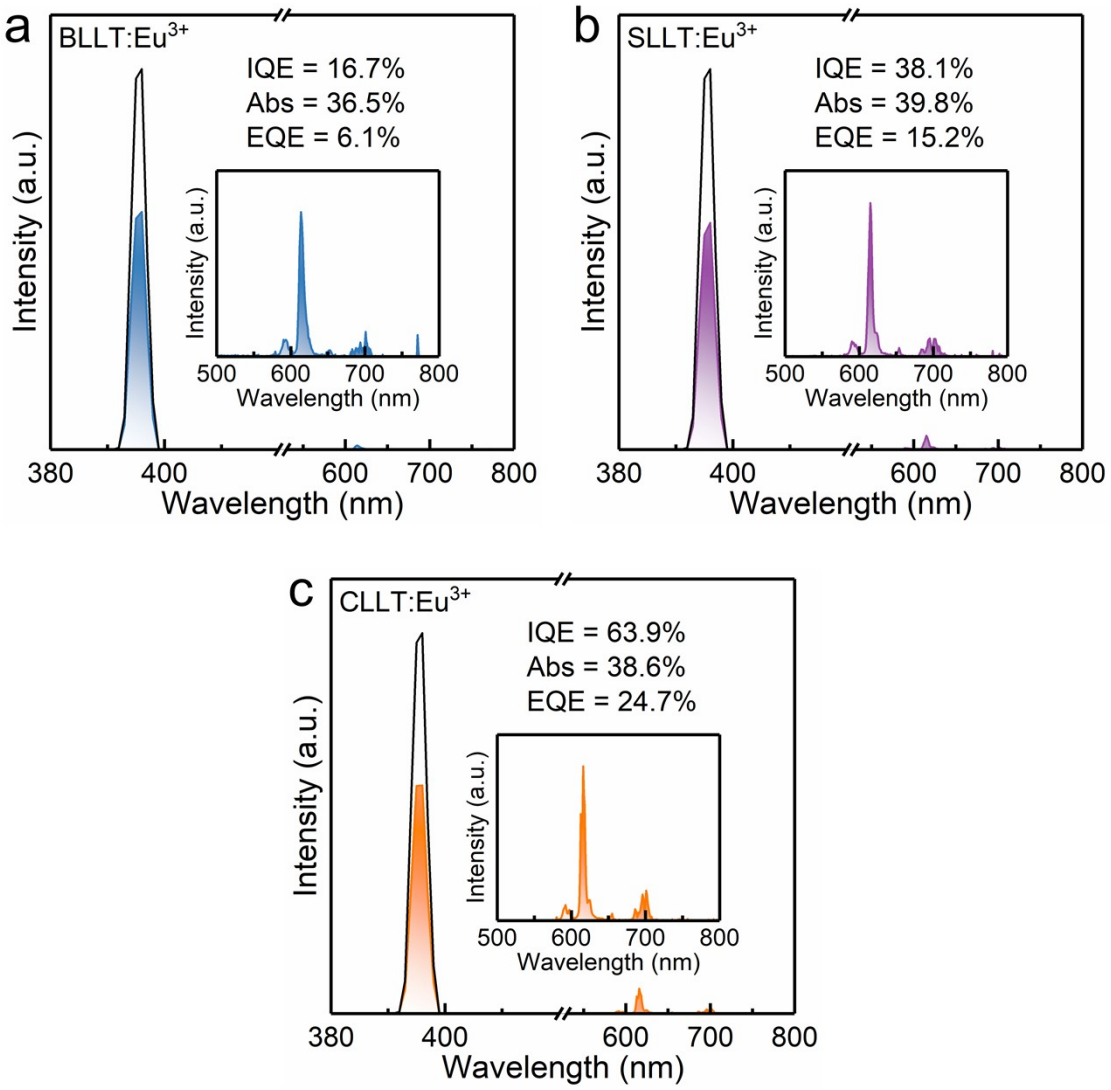

Figure S9. Quantum efficiency and absorption factor determination details of (a) BLLT:Eu^{3+}, (b) SLLT:Eu^{3+} and (c) CLLT:Eu^{3+}.

Table S1. Fractional atomic coordinates, occupancy factors, isotropic displacement parameters (Å^2) and main parameters of processing of the refinements of XLLT:Eu^{3+}.

(a) BLLT:Eu^{3+}

Atom	Wyckoff position	*x*	*y*	*z*	Occ.	$U_{iso} \times 100$
Ba	4e	0.4995(5)	0.5026(4)	0.2542(9)	0.5	2.69(6)
La	4e	0.4995(5)	0.5026(4)	0.2542(9)	0.35	2.69(6)
Eu	4e	0.4995(5)	0.5026(4)	0.2542(9)	0.15	2.69(6)
Li	2d	1/2	0	0	1	2
Te	2a	0	1/2	0	1	2.59(7)
O1	4e	0.2003(6)	0.1854(4)	0.0017(4)	1	5.78(3)
O2	4e	0.2161(7)	0.7792(1)	0.0074(7)	1	5.24(8)
O3	4e	0.5334(7)	-0.0022(4)	0.2408(1)	1	5.25(0)

Space group:$P2_1/n$ (*No.*14), Monoclinic. a = 5.7098(0) Å, b = 5.6878(5) Å, c = 8.0466(8) Å, β = 89.8810 °, R_{wp} = 7.5%, R_p = 5.4%, χ^2 = 1.84.

(b) SLLT:Eu^{3+}

Atom	Wyckoff position	*x*	*y*	*z*	Occ.	$U_{iso} \times 100$
Sr	4e	0.4984(0)	0.5156(3)	0.2504(5)	0.5	3.35(6)
La	4e	0.4984(0)	0.5156(3)	0.2504(5)	0.35	3.35(6)
Eu	4e	0.4984(0)	0.5156(3)	0.2504(5)	0.15	3.35(6)
Li	2d	1/2	0	0	1	2
Te	2a	0	1/2	0	1	3.67(2)
O1	4e	0.2080(6)	0.2440(6)	-0.0324(7)	1	5.20(3)
O2	4e	0.2790(5)	0.7132(5)	0.0199(6)	1	3.71(7)
O3	4e	0.5350(7)	0.0202(5)	0.2280(7)	1	5.32(5)

Space group:$P2_1/n$ (*No.*14), Monoclinic. a = 5.6300(0) Å, b = 5.5926(2) Å, c = 7.9329(1) Å, β = 90.0841 °, R_{wp} = 8.7%, R_p = 6.2%, χ^2 = 3.85.

(c) CLLT:Eu^{3+}

Atom	Wyckoff position	*x*	*y*	*z*	Occ.	$U_{iso} \times 100$
Ca	4e	0.5018(7)	0.5240(3)	0.2417(9)	0.5	2.74(7)
La	4e	0.5018(7)	0.5240(3)	0.2417(9)	0.35	2.74(7)
Eu	4e	0.5018(7)	0.5240(3)	0.2417(9)	0.15	2.74(7)
Li	2d	1/2	0	0	1	2
Te	2a	0	1/2	0	1	3.38(4)

O1	4e	0.1296(0)	0.3082(7)	0.0961(9)	1	5.75(5)
O2	4e	0.2261(2)	0.7933(6)	0.0117(4)	1	3.31(9)
O3	4e	0.6005(6)	-0.0833(0)	0.1435(1)	1	4.84(2)

Space group:$P2_1/n$ (*No.*14), Monoclinic. a = 5.6377(5) Å, b = 5.5437(8) Å, c = 7.8617(8) Å, β = 90.0018 °, R_{wp} = 7.4%, R_p = 5.5%, χ^2 = 1.94.

(d) MLLT:Eu^{3+}

Atom	Wyckoff position	x	y	z	Occ.	$U_{iso} \times 100$
Mg	4e	0.4944(6)	0.5159(1)	0.2523(1)	0.5	2.63(9)
La	4e	0.4944(6)	0.5159(1)	0.2523(1)	0.35	2.63(9)
Eu	4e	0.4944(6)	0.5159(1)	0.2523(1)	0.15	2.63(9)
Li	2d	1/2	0	0	1	2
Te	2a	0	1/2	0	1	2.78(9)
O1	4e	0.2401(4)	0.0980(1)	-0.0035(1)	1	5.85(8)
O2	4e	0.1994(7)	0.7864(1)	0.0149(8)	1	3.02(3)
O3	4e	0.5341(3)	0.0267(9)	0.2568(8)	1	3.84(2)

Space group:$P2_1/n$ (*No.*14), Monoclinic. a = 5.5483(2) Å, b = 5.5466(4) Å, c = 7.8623(5) Å, β = 89.8228 °, R_{wp} = 8.1%, R_p = 5.7%, χ^2 = 2.32.

Table S2. The ionic radii of the cations in the different folds of coordination.

Ion	Coordination	Ionic radii (Å)
Mg^{2+}	6	0.72
La^{3+}	7	1.10
Eu^{3+}	7	1.01
Li^{+}	6	0.76
Te^{6+}	6	0.56

Table S3. Electroluminescence properties of blue-emitting $Na_{1.3}Hf_{1.7}Sc_{0.3}(PO_4)_3:Eu^{2+}$, yellow-emitting Ba, $Sr)_2SiO_4:Eu^{2+}$ and red-emitting MLLT:Eu^{3+} phosphors and 395 nm n-UV LED chip based white-LED device under various currents.

Current (mA)	Coordinate (x, y)	CCT (K)	CRI (R_a)	Luminous efficacy (lm · W^{-1})

50	(0.4236, 0.4197)	3357	88.1	15.31
100	(0.4217, 0.4197)	3402	88.2	15.61
150	(0.4198, 0.4199)	3432	88.4	15.11
200	(0.4170, 0.4204)	3490	89.1	14.51
250	(0.4156, 0.4206)	3516	89.2	14.21
300	(0.4146, 0.4206)	3537	89.3	13.91
350	(0.4086, 0.4186)	3643	89.8	12.61