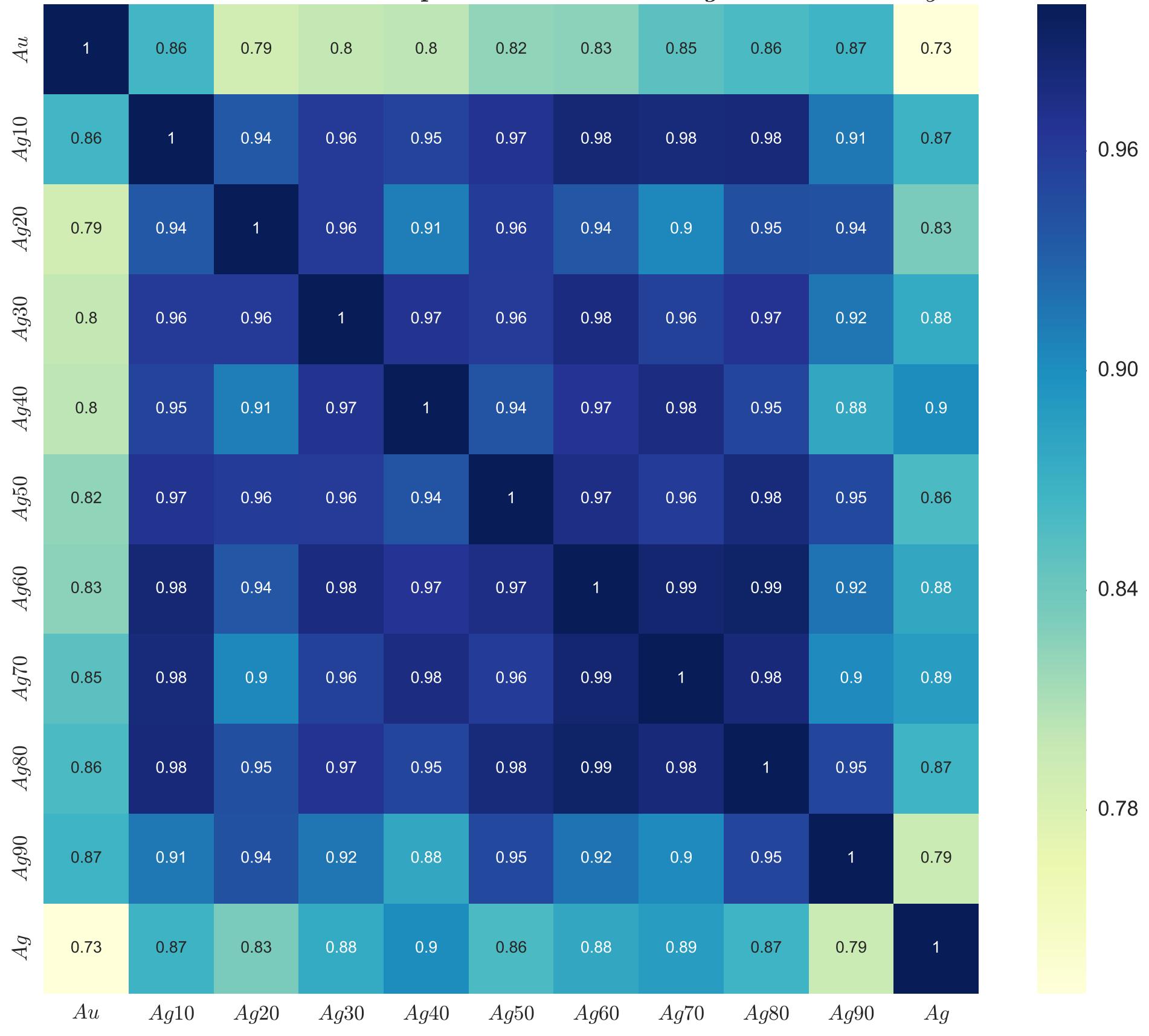
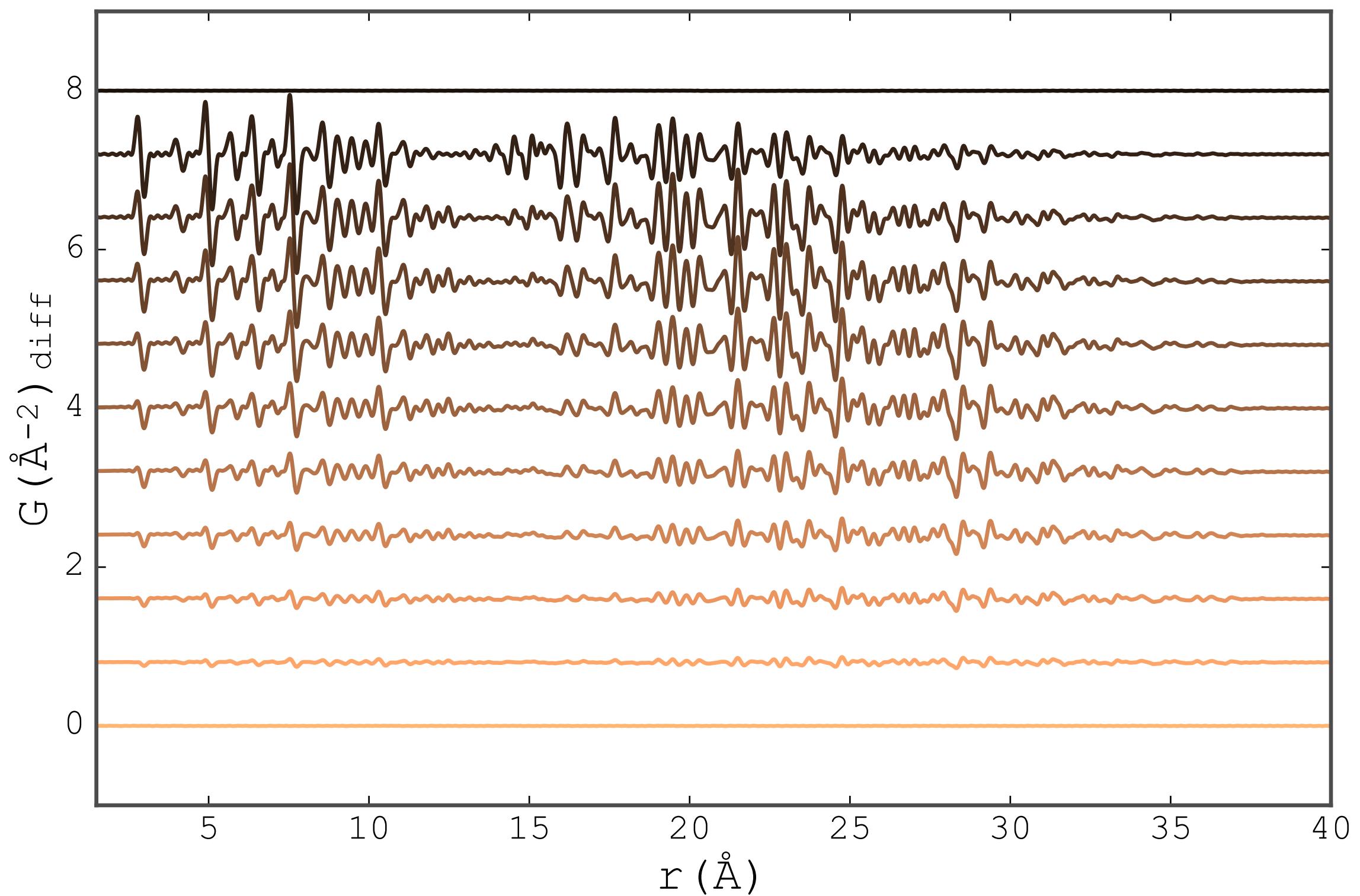
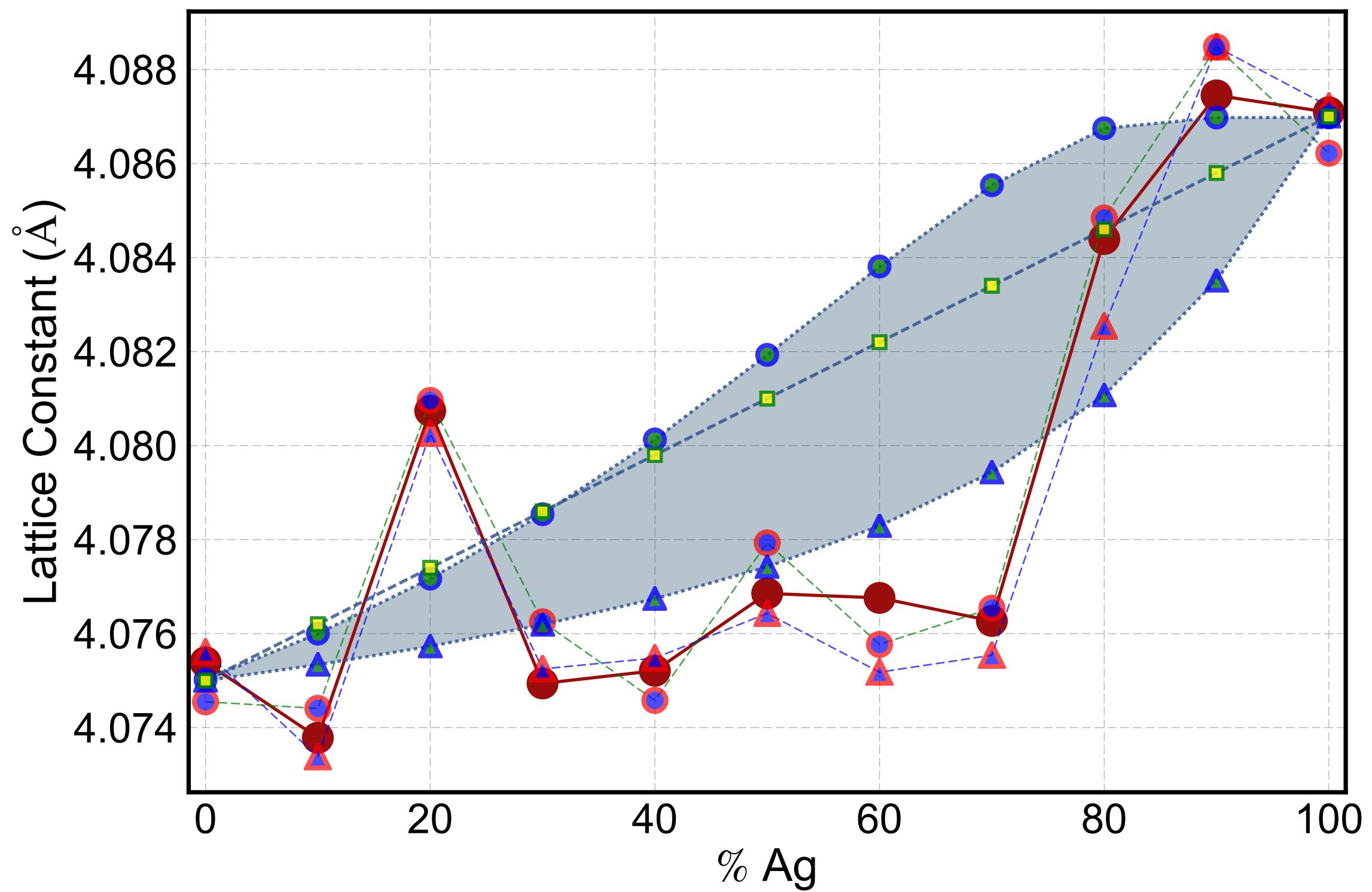
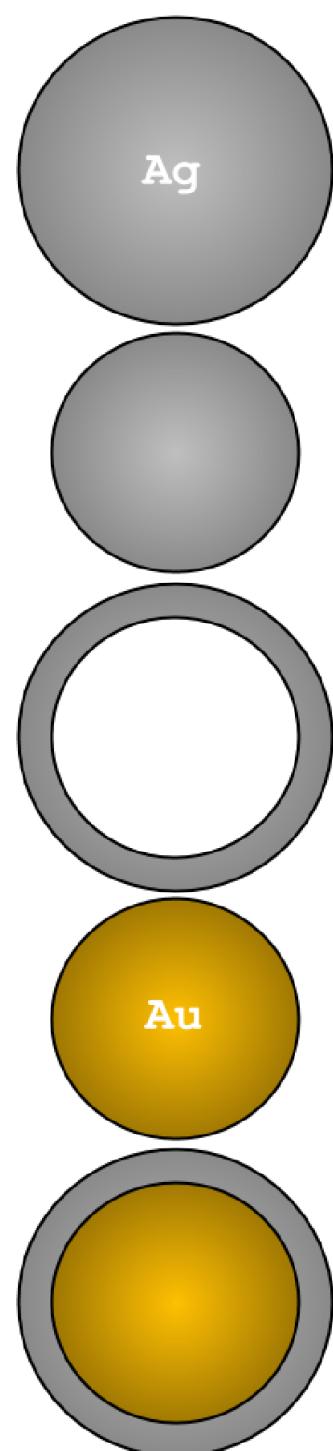
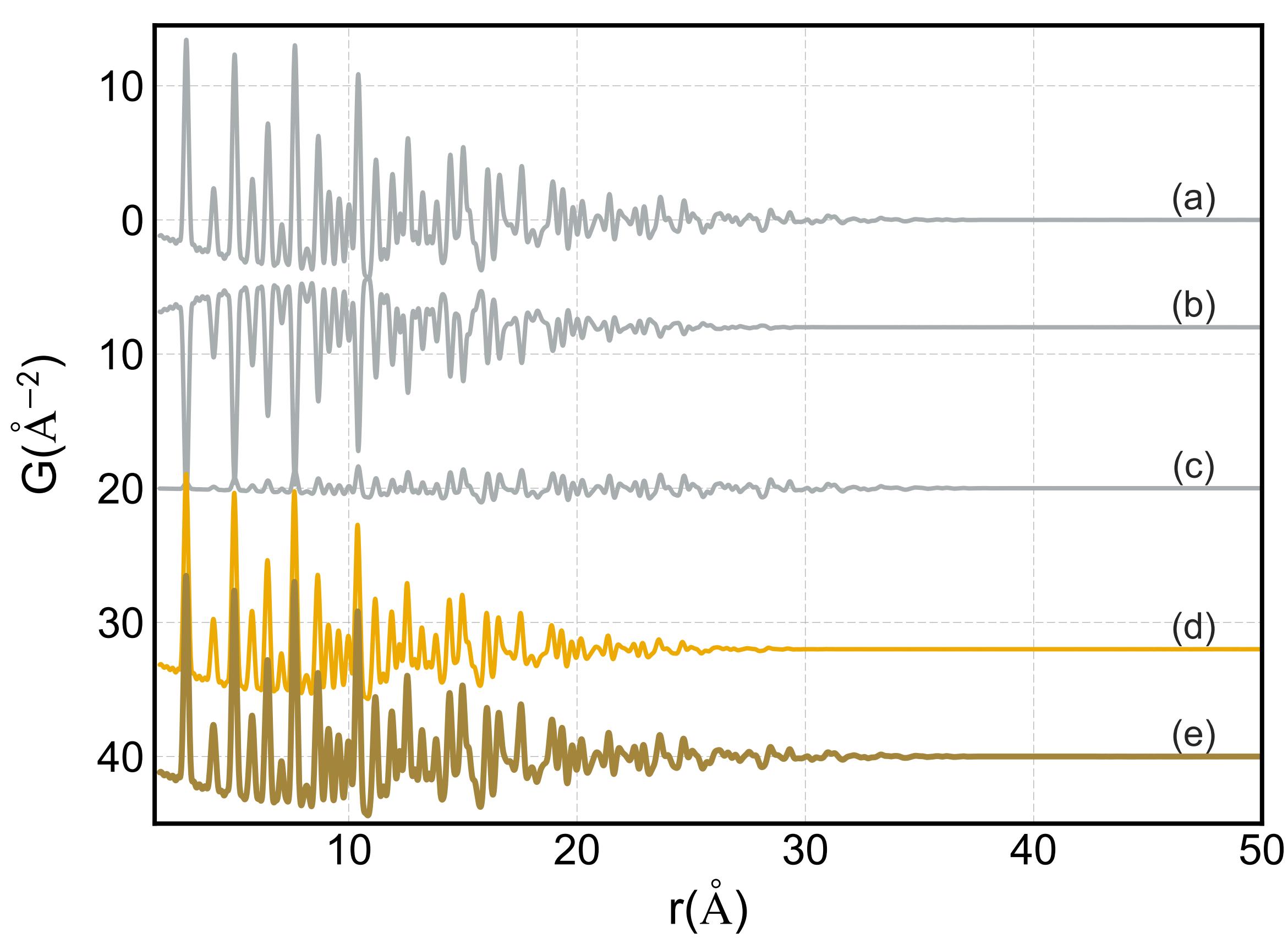


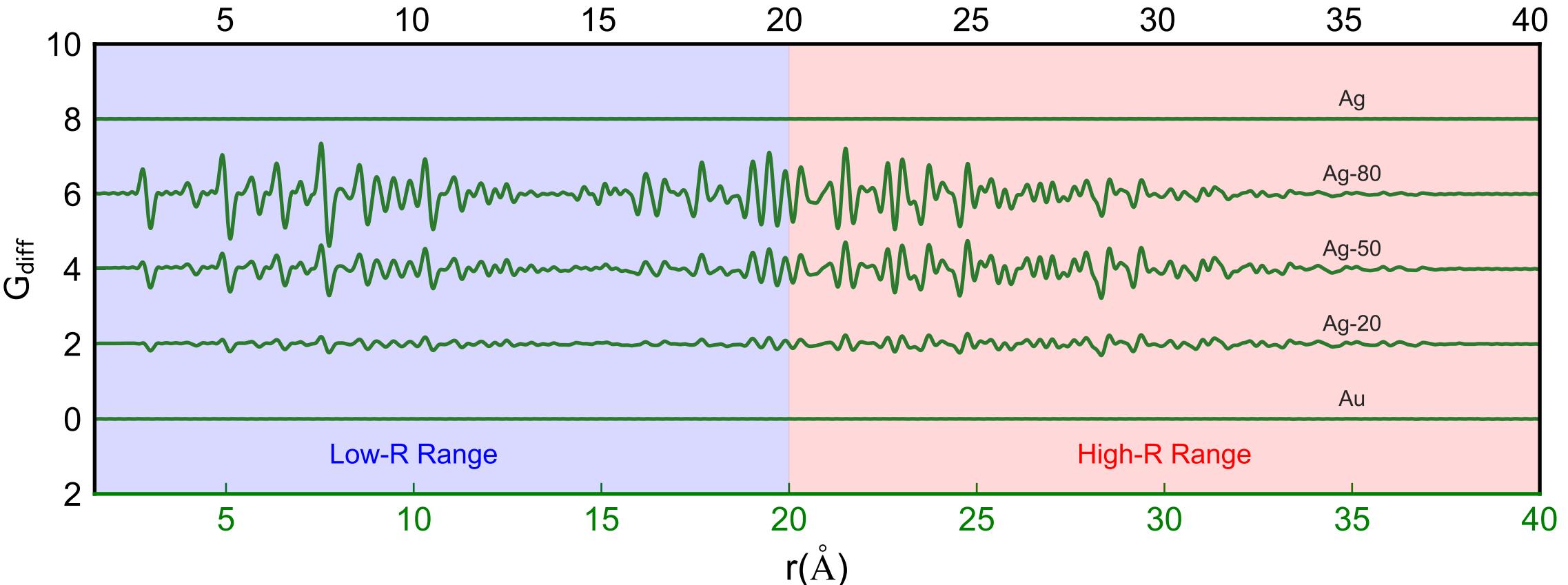
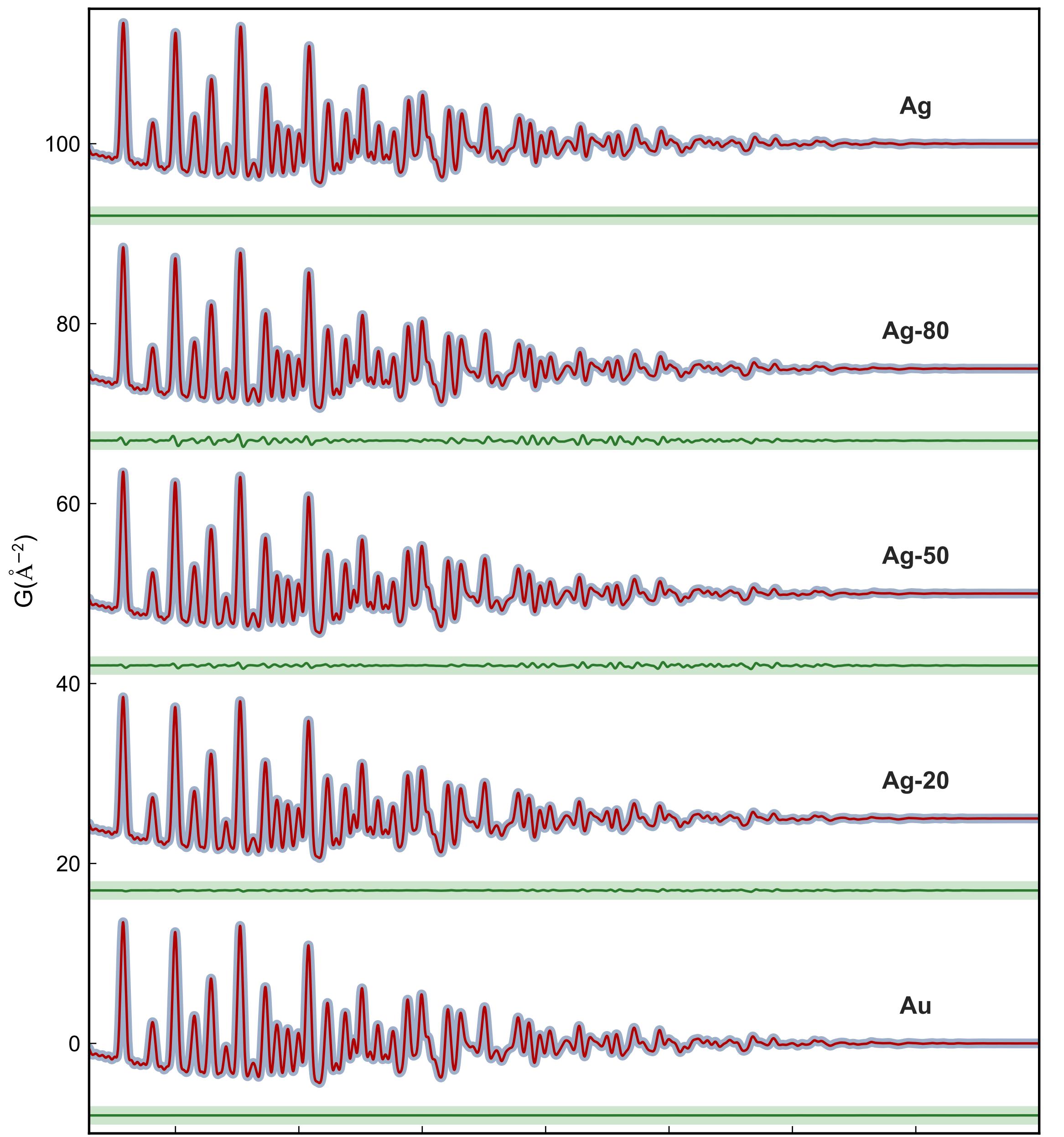
Pearson Correlation Map : FitResiduals – AgAu – FCCAlloy

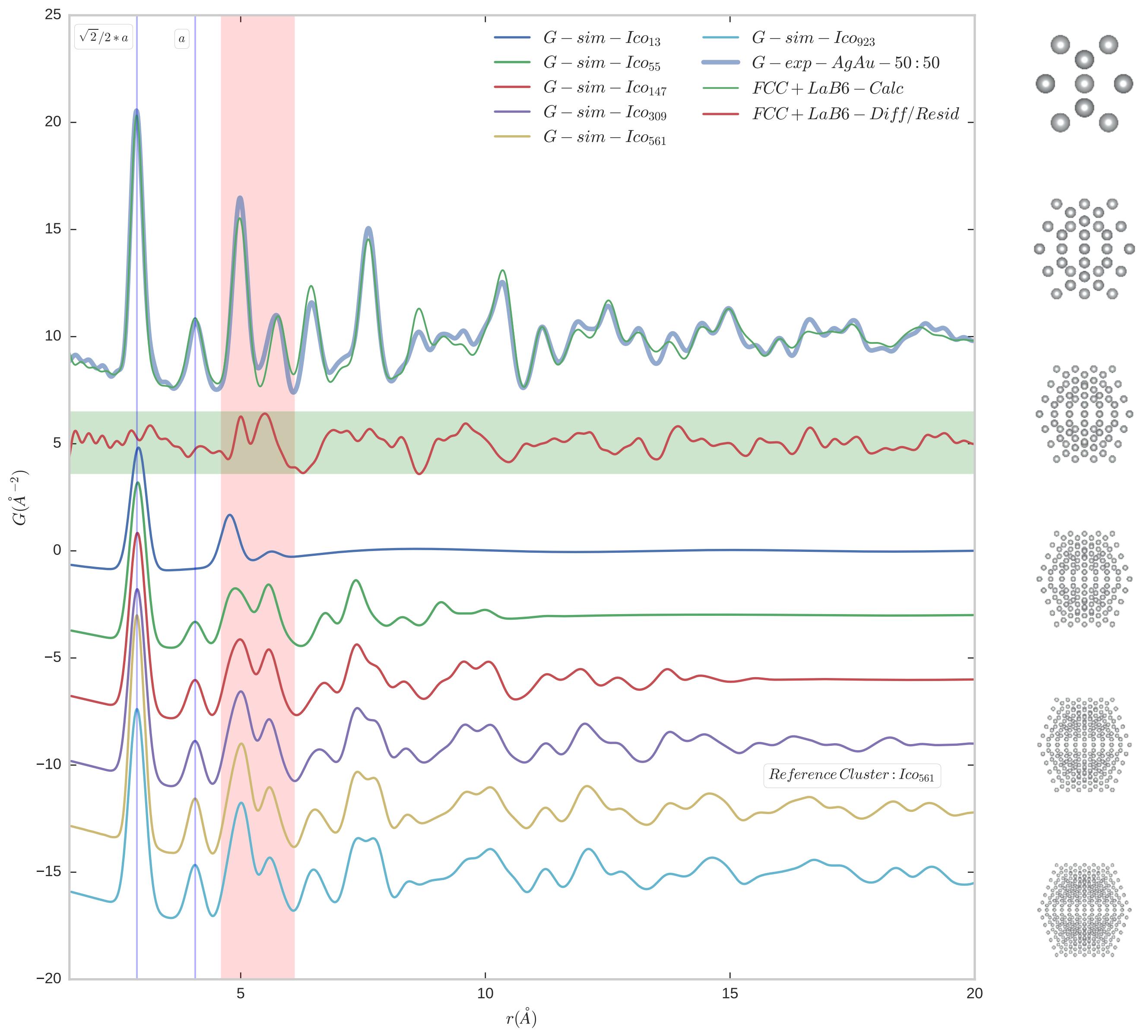


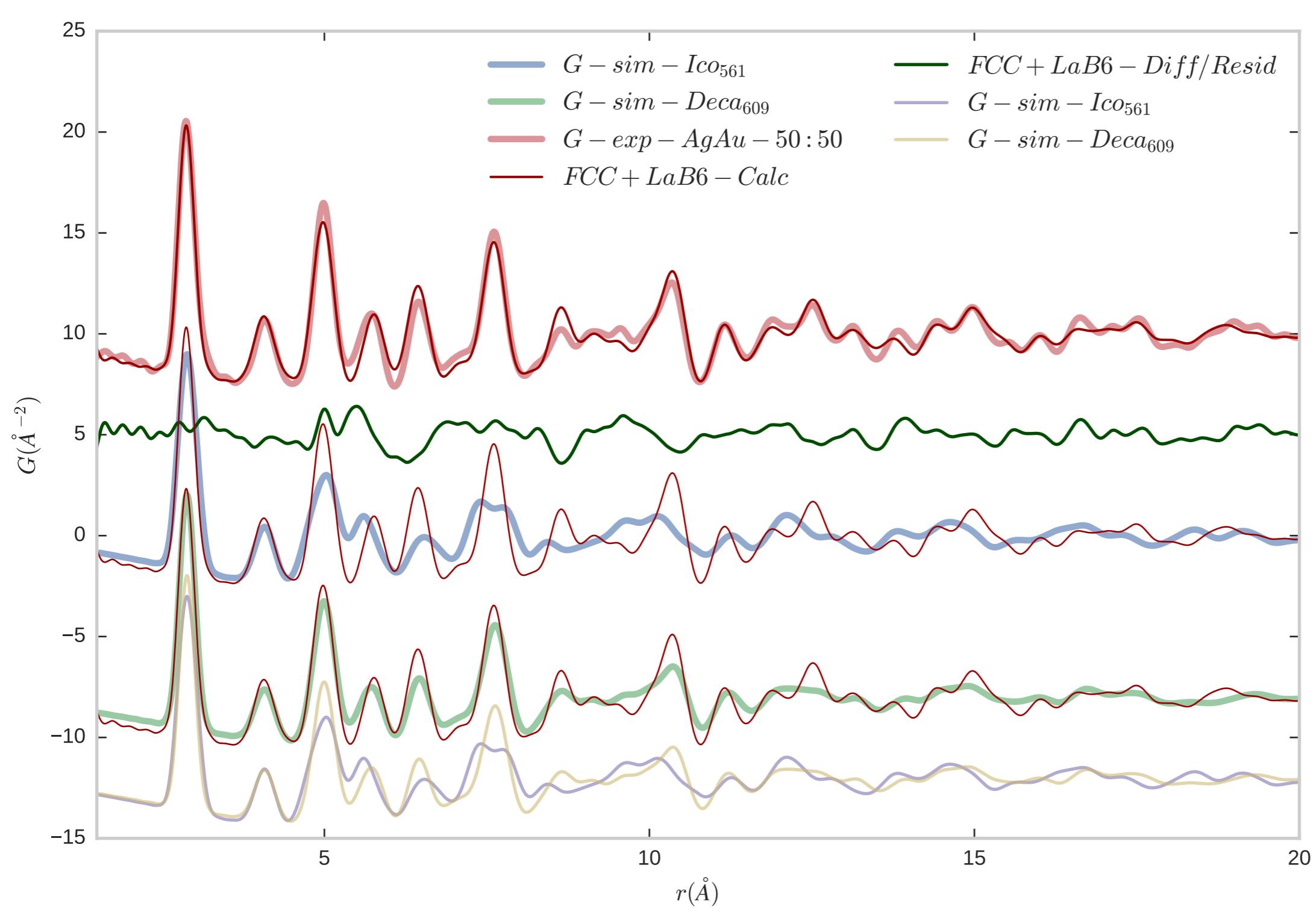




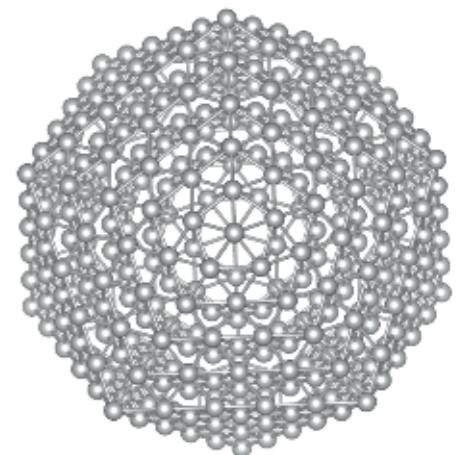




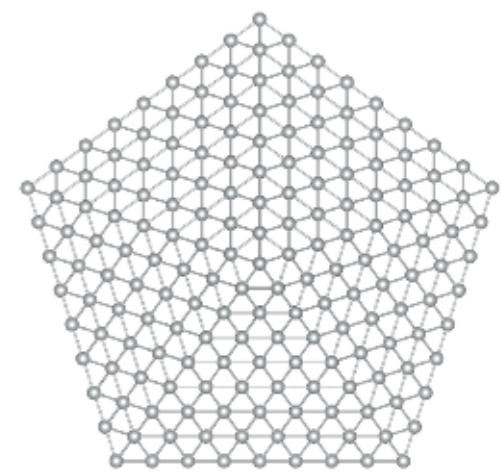




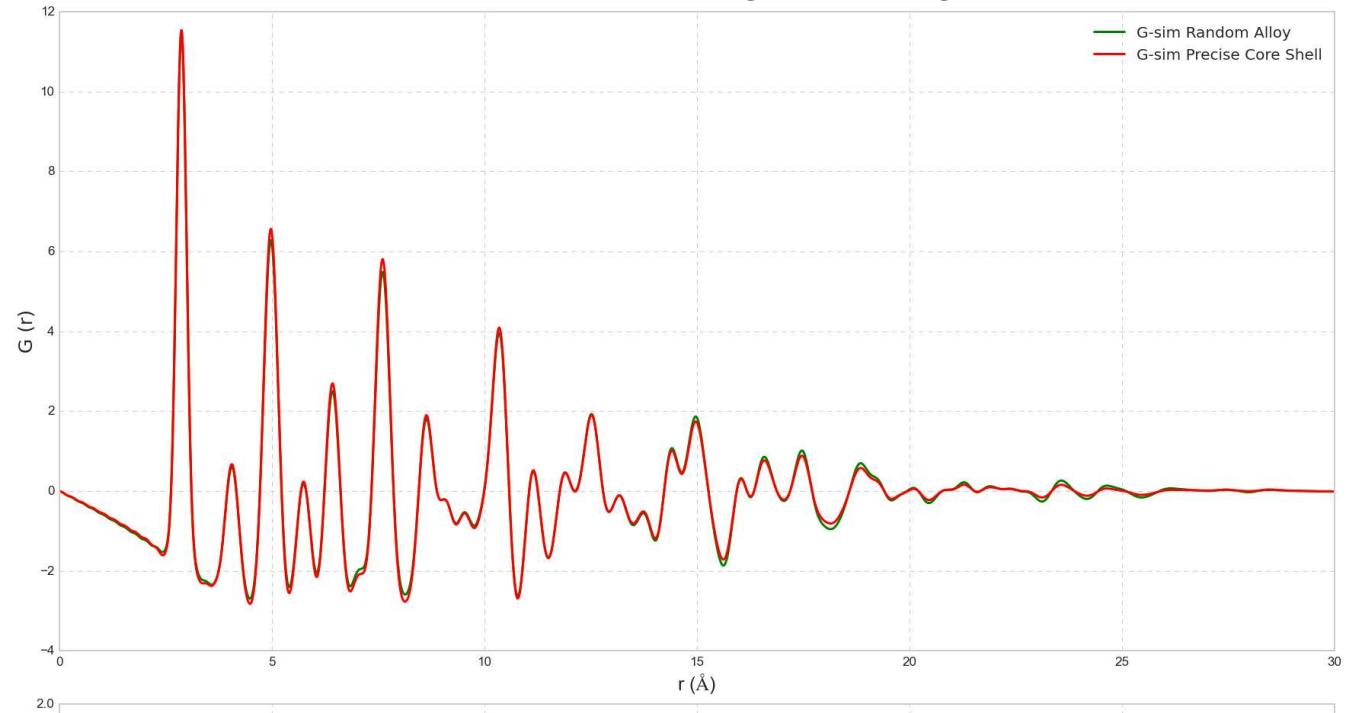
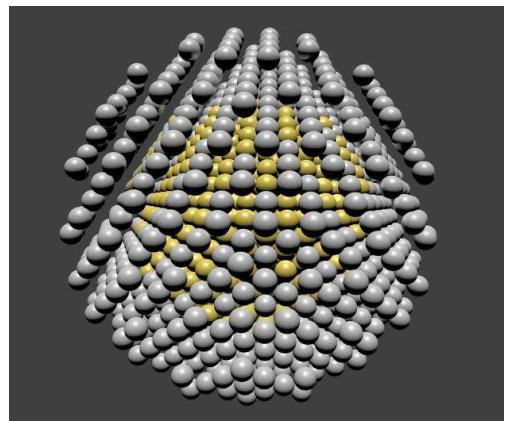
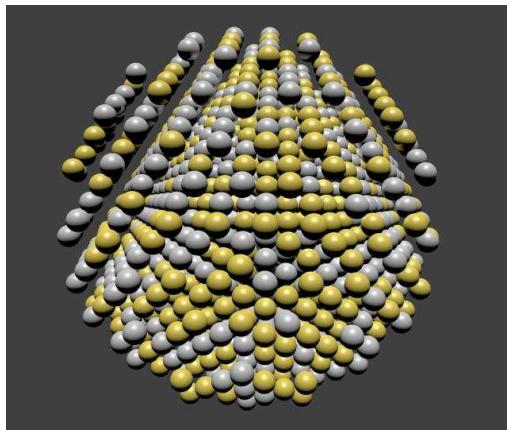
$Ico_{561}$



$Marks_{609} - 9 - 9 - 9$



## Discrete NP Modeling: A Learning Exercise



$$Volume_{core} = \frac{4}{3}\pi r_{Au}^3$$

$$Volume_{shell} = \frac{4}{3}\pi(R_{Ag}^3 - r_{Au}^3)$$

$$\frac{Volume_{core}}{Volume_{shell}} = Composition = \frac{r_{Au}^3}{R_{Ag}^3 - r_{Au}^3}$$

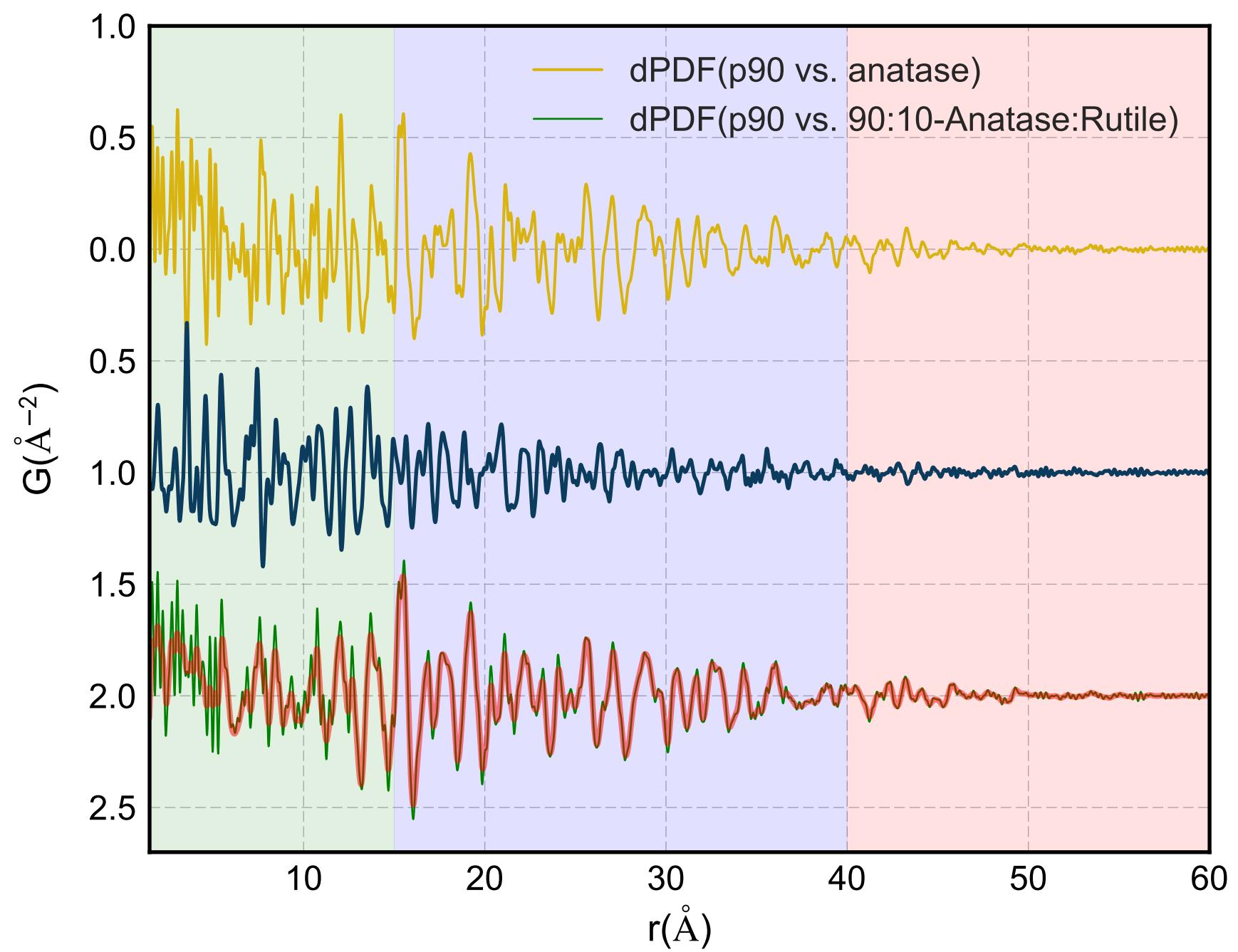
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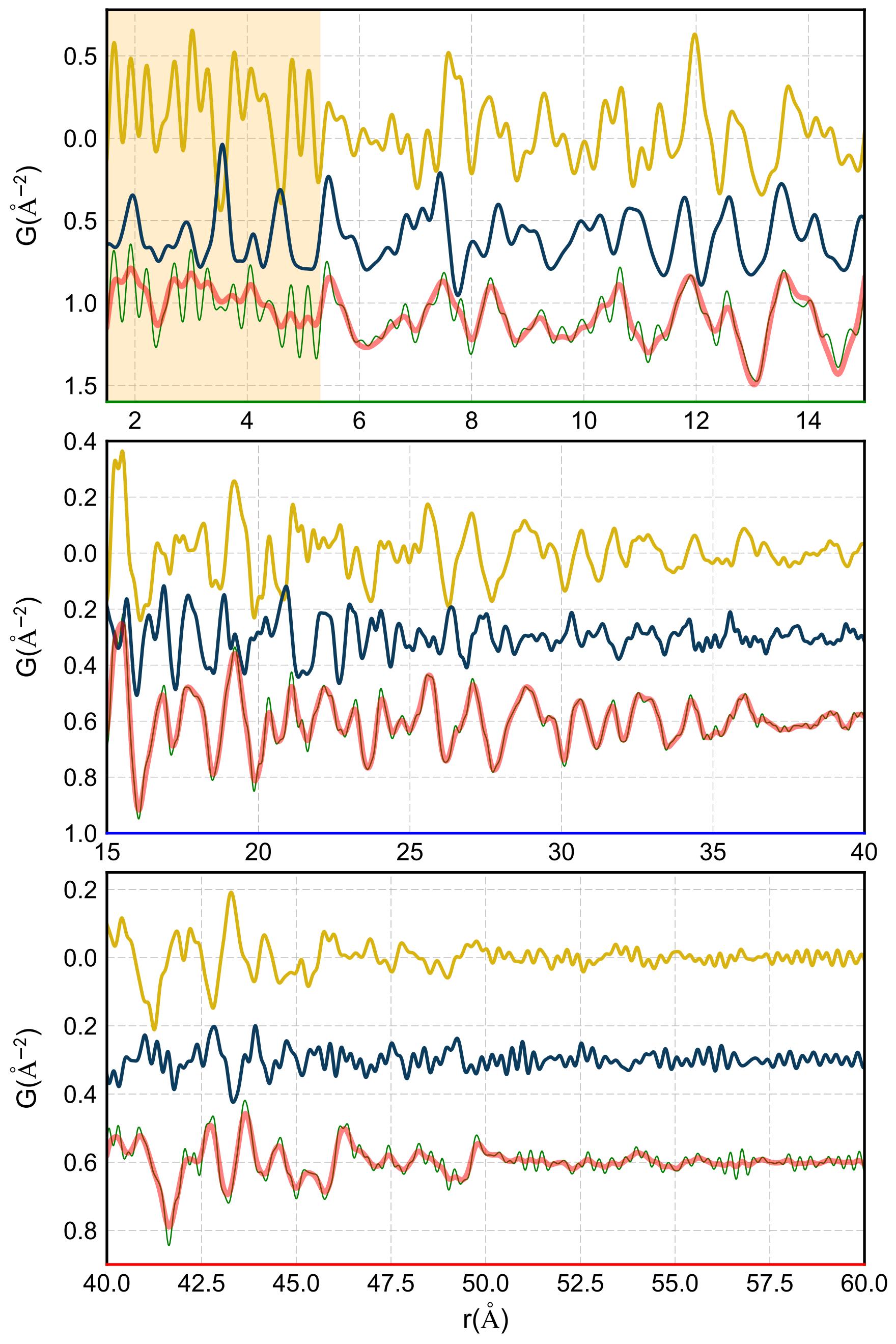

$$r_{Au} = \left( \frac{R_{Ag} \times Composition}{1 + Composition} \right)^{\frac{1}{3}} = \left( \frac{R_{NP} \times Composition}{1 + Composition} \right)^{\frac{1}{3}}$$

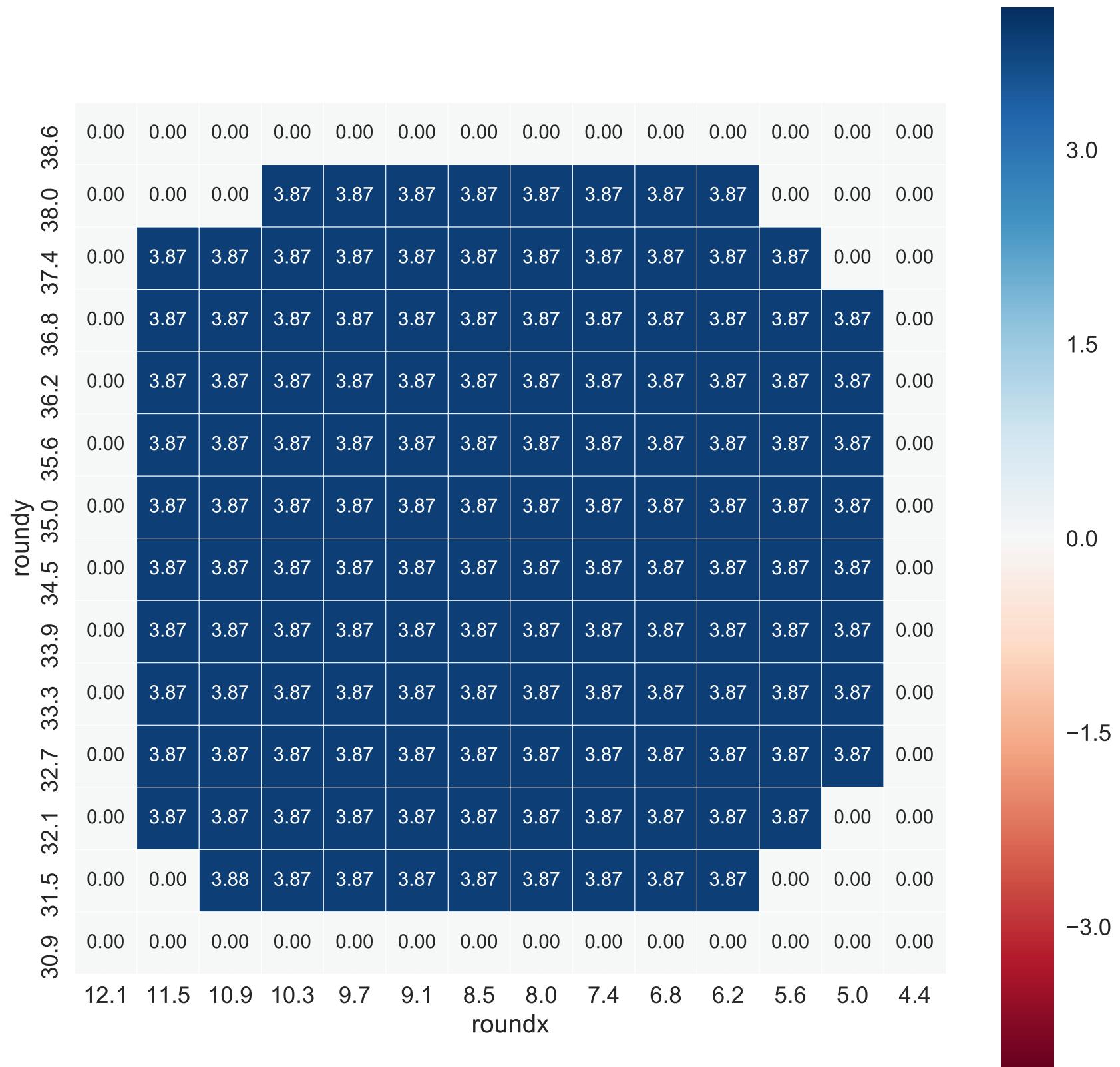

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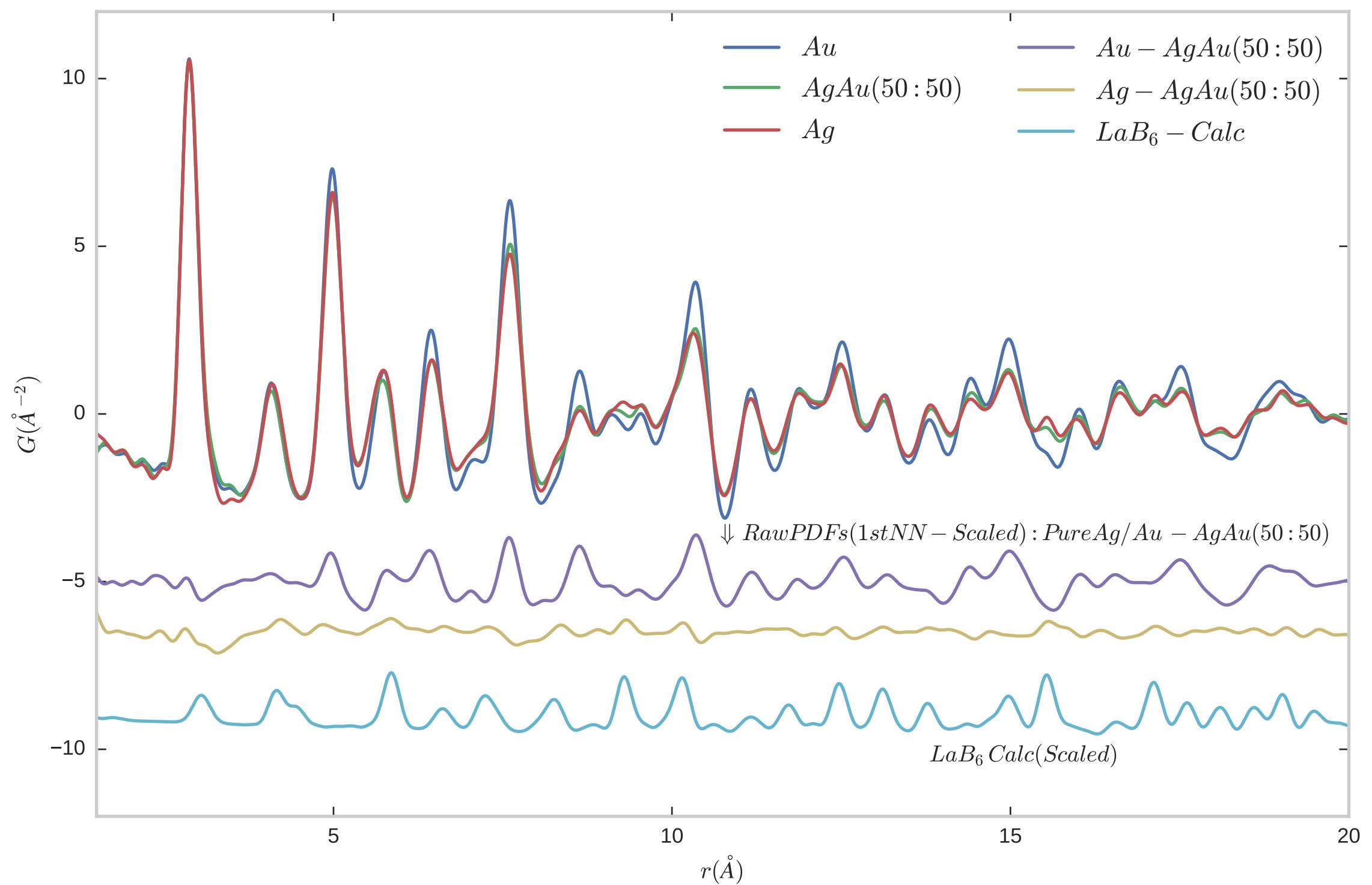
$$R_{NP} \equiv R_{Ag}$$

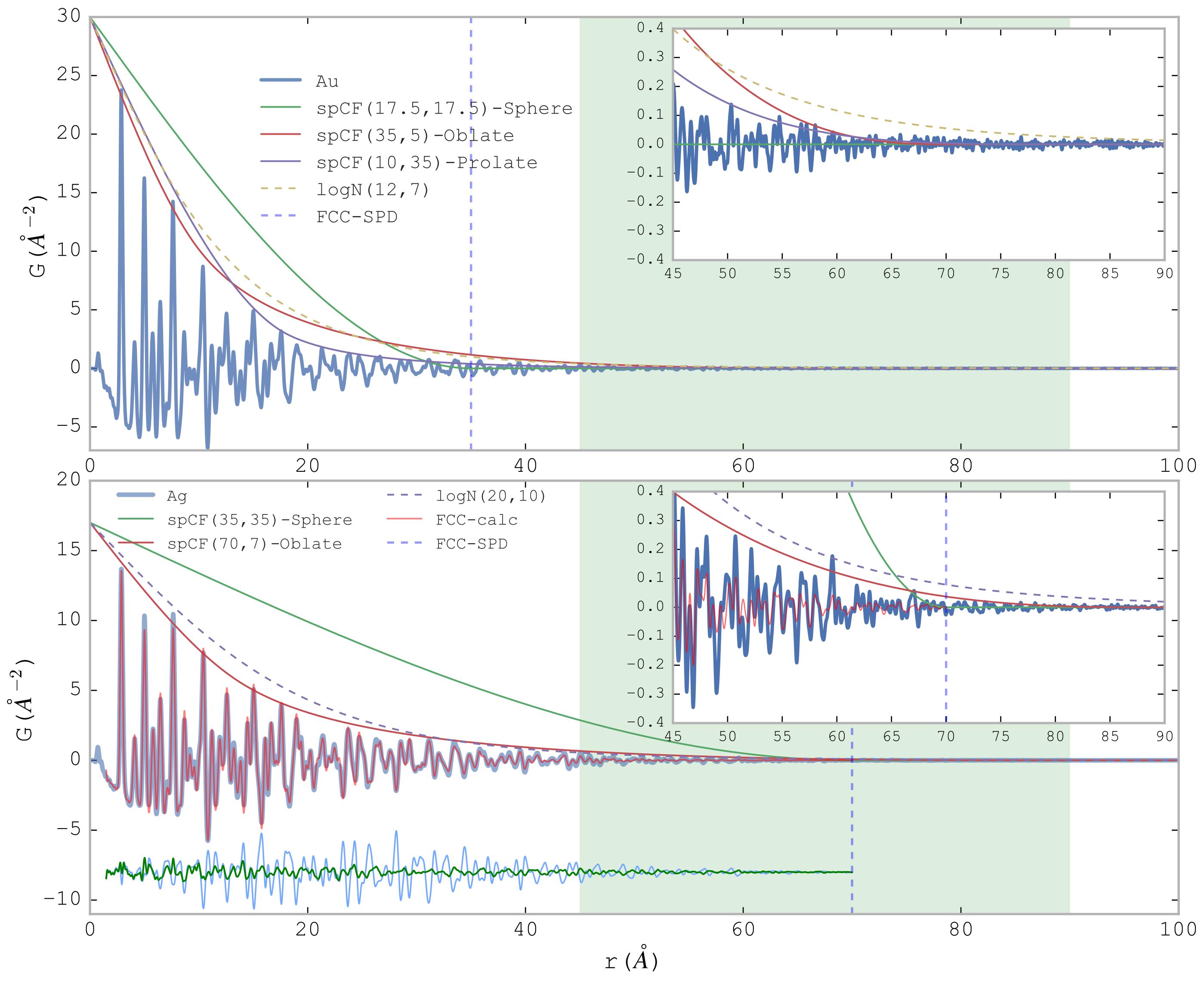
$$R_{Shell} \equiv R_{NP} - R_{Au} = R_{NP} - r_{Au}$$



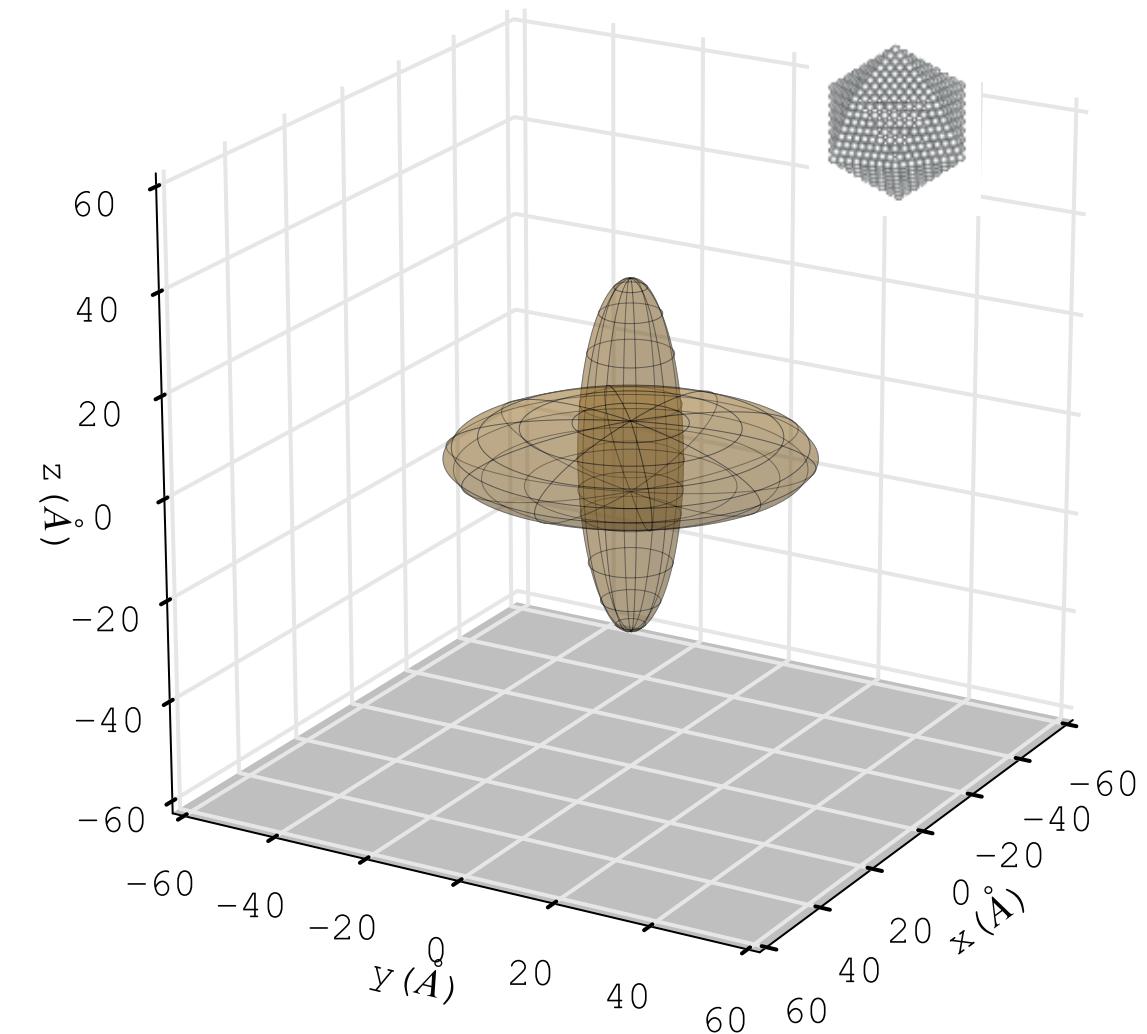




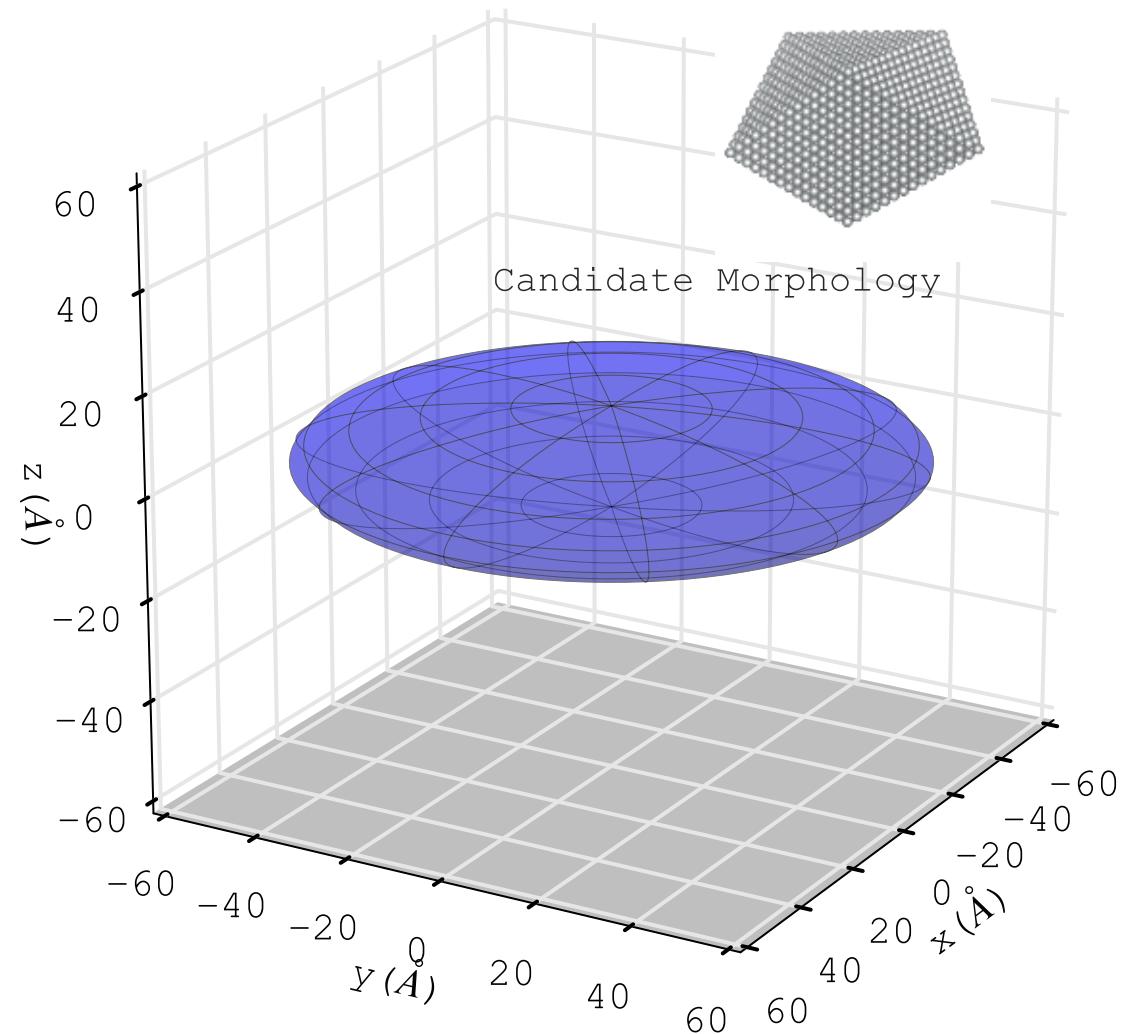


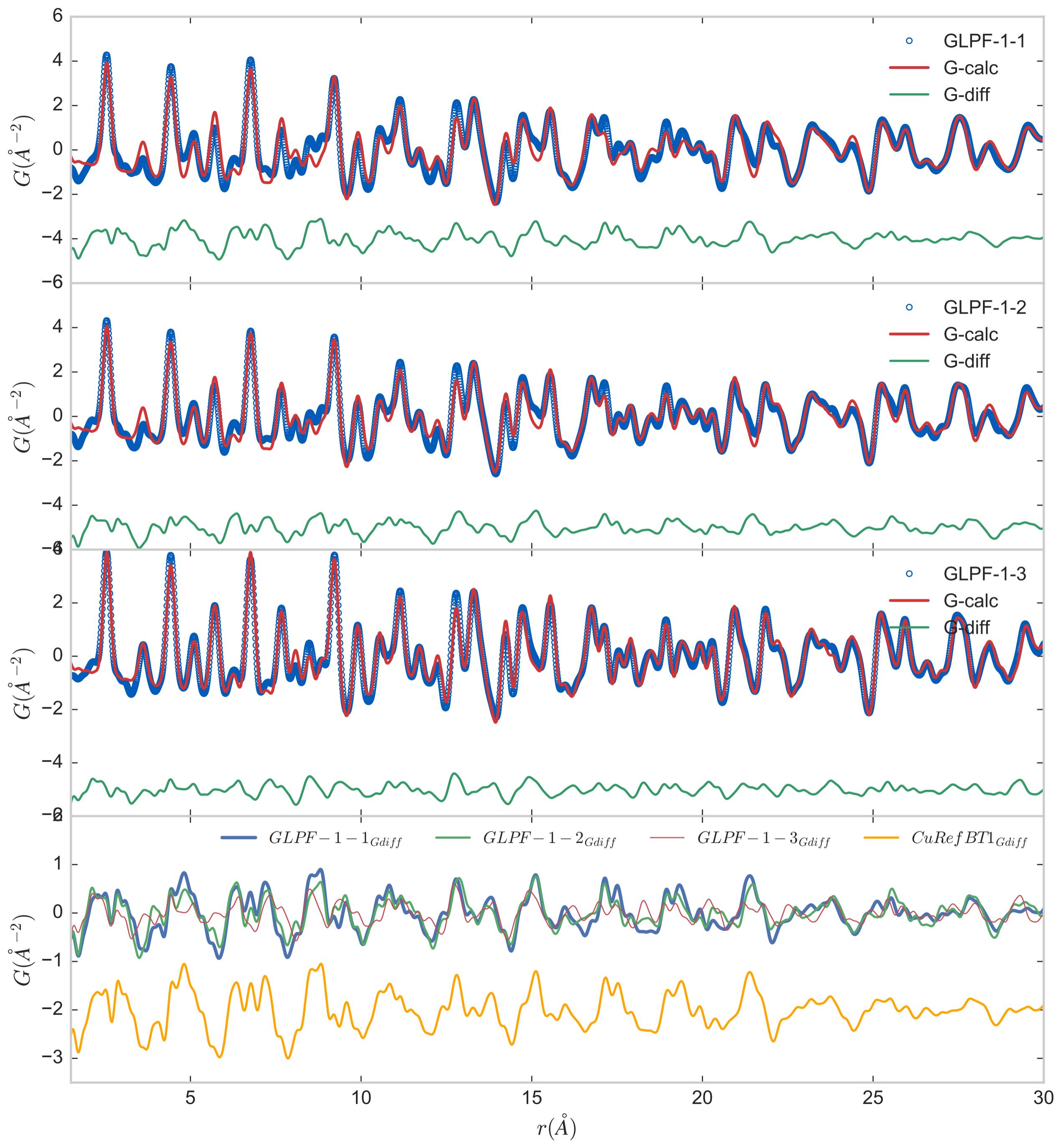


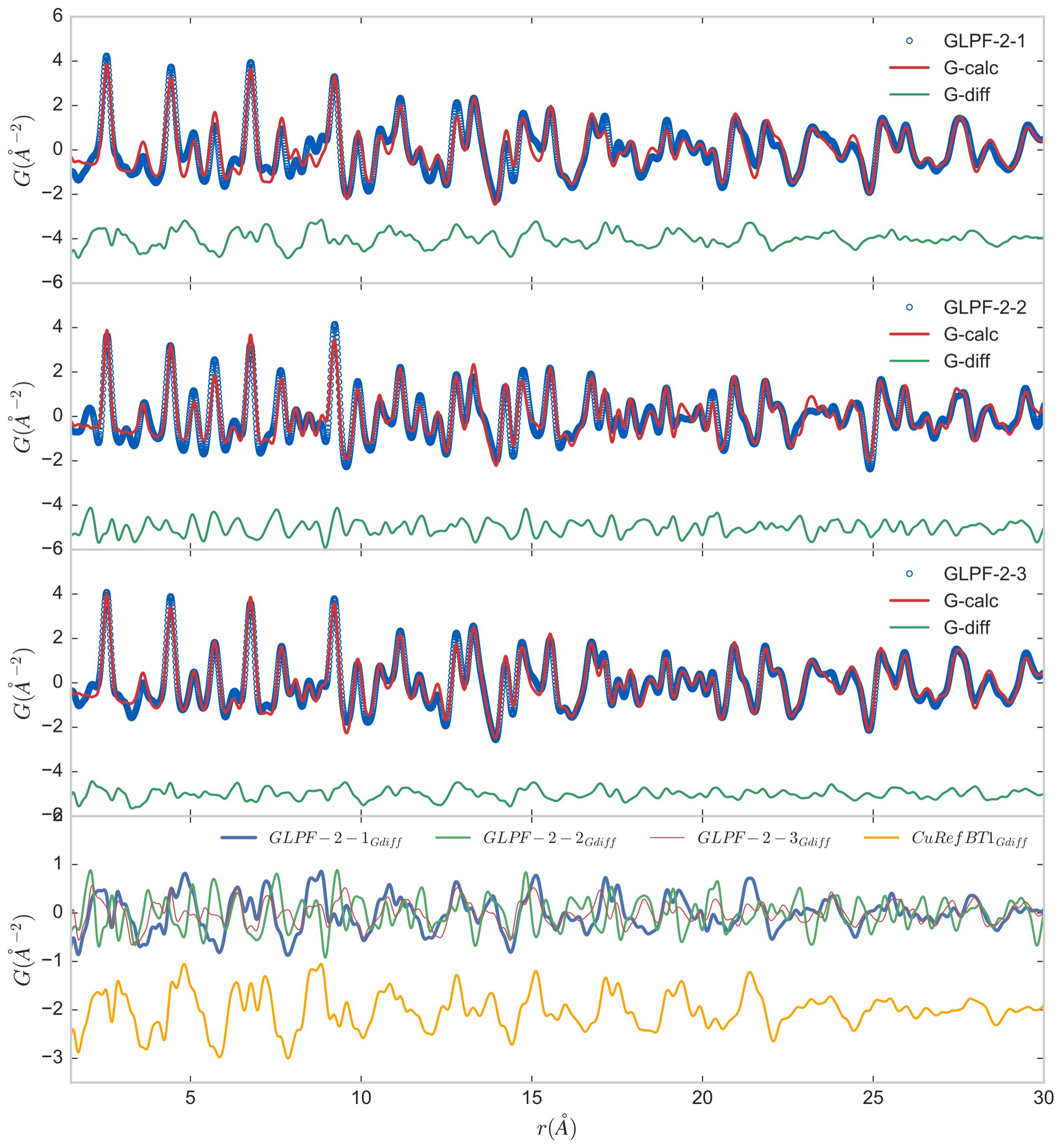
Au Form Factor (Oblate+Prolate)

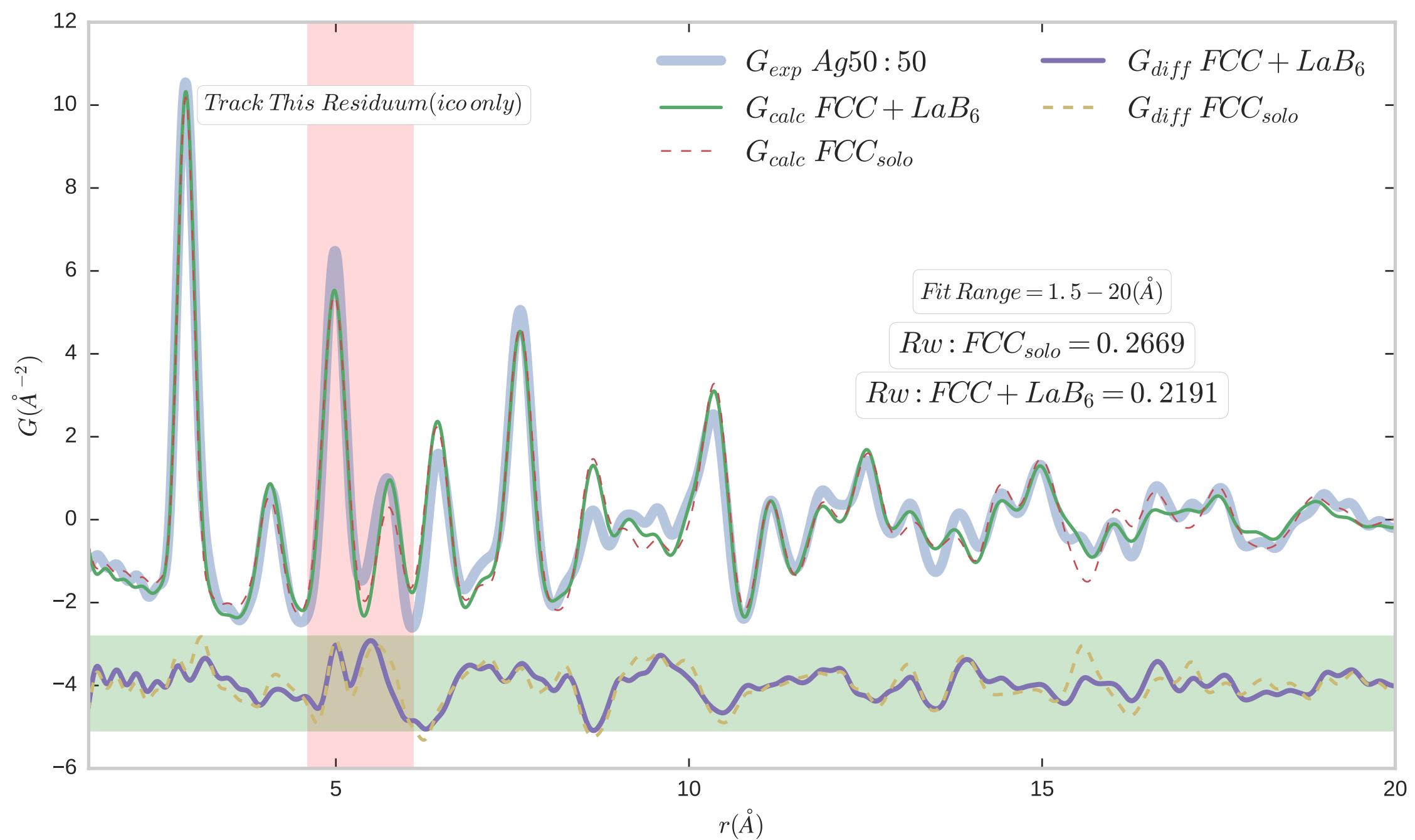


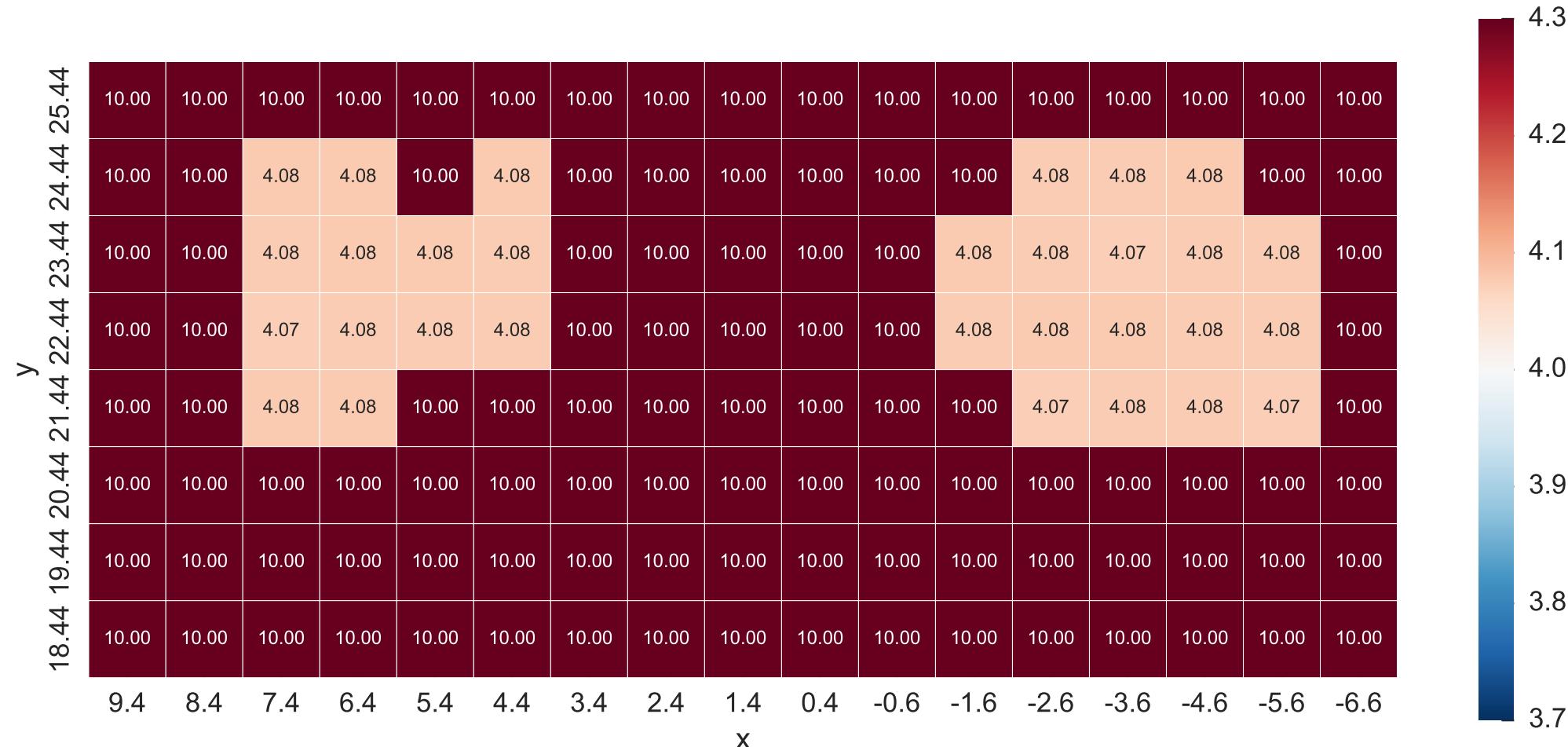
Ag Form Factor (Oblate)

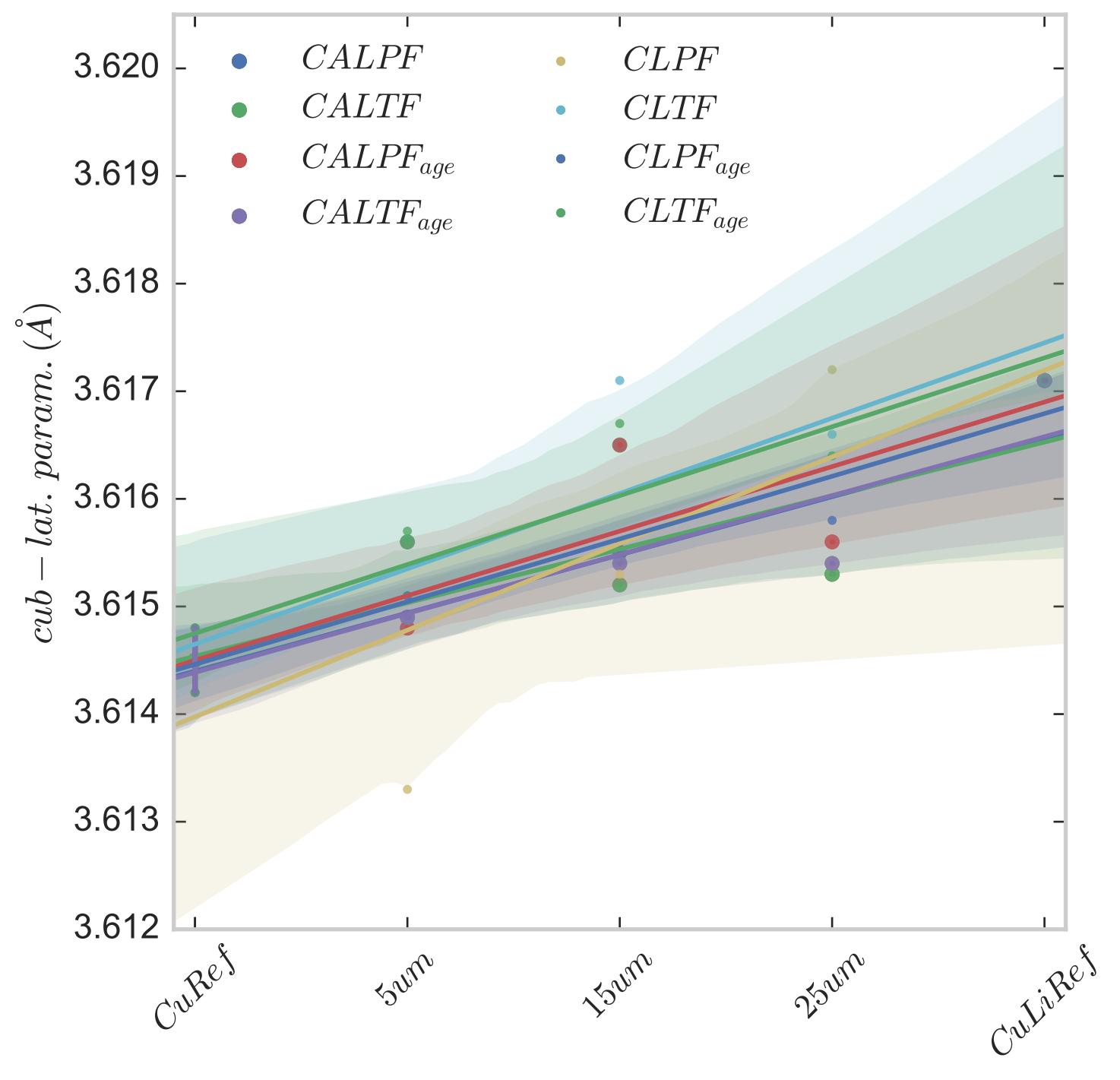


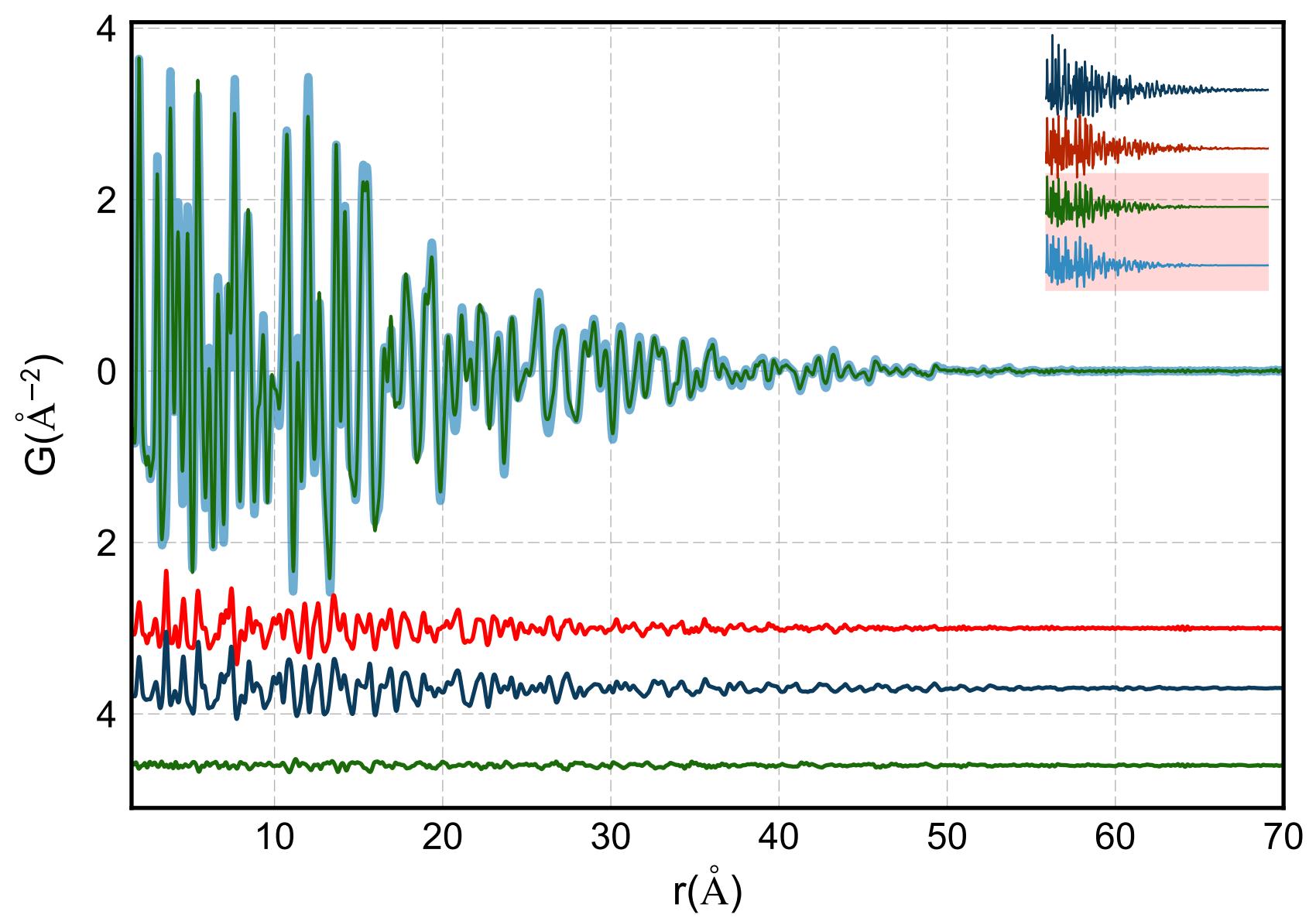


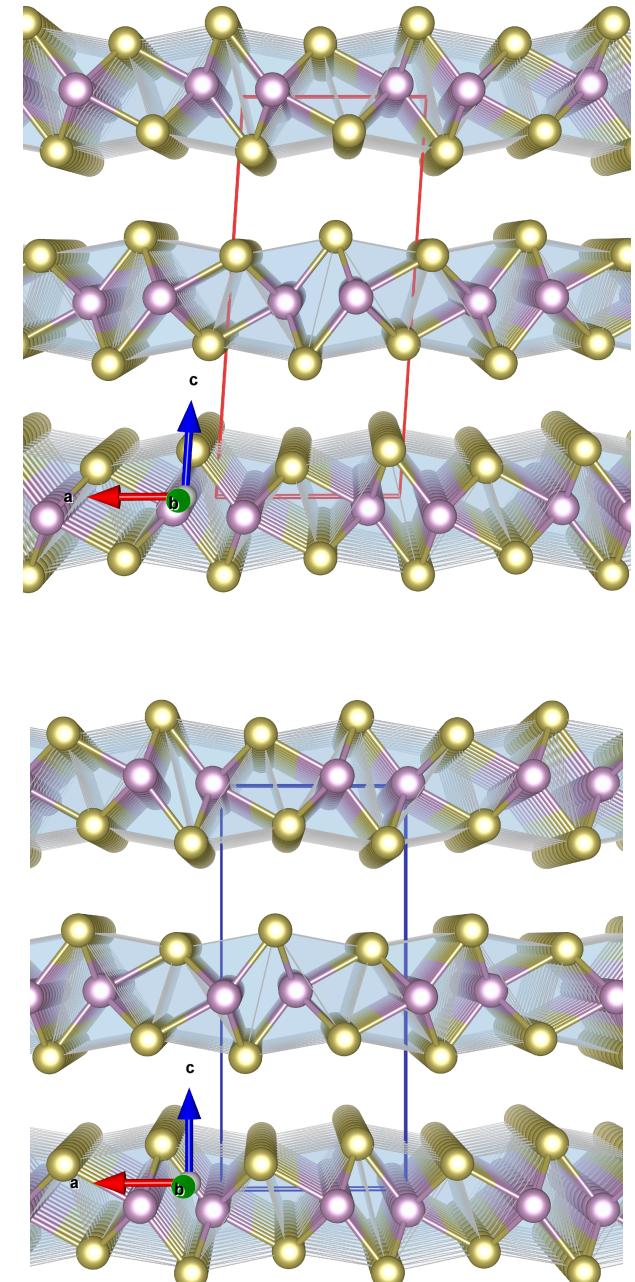
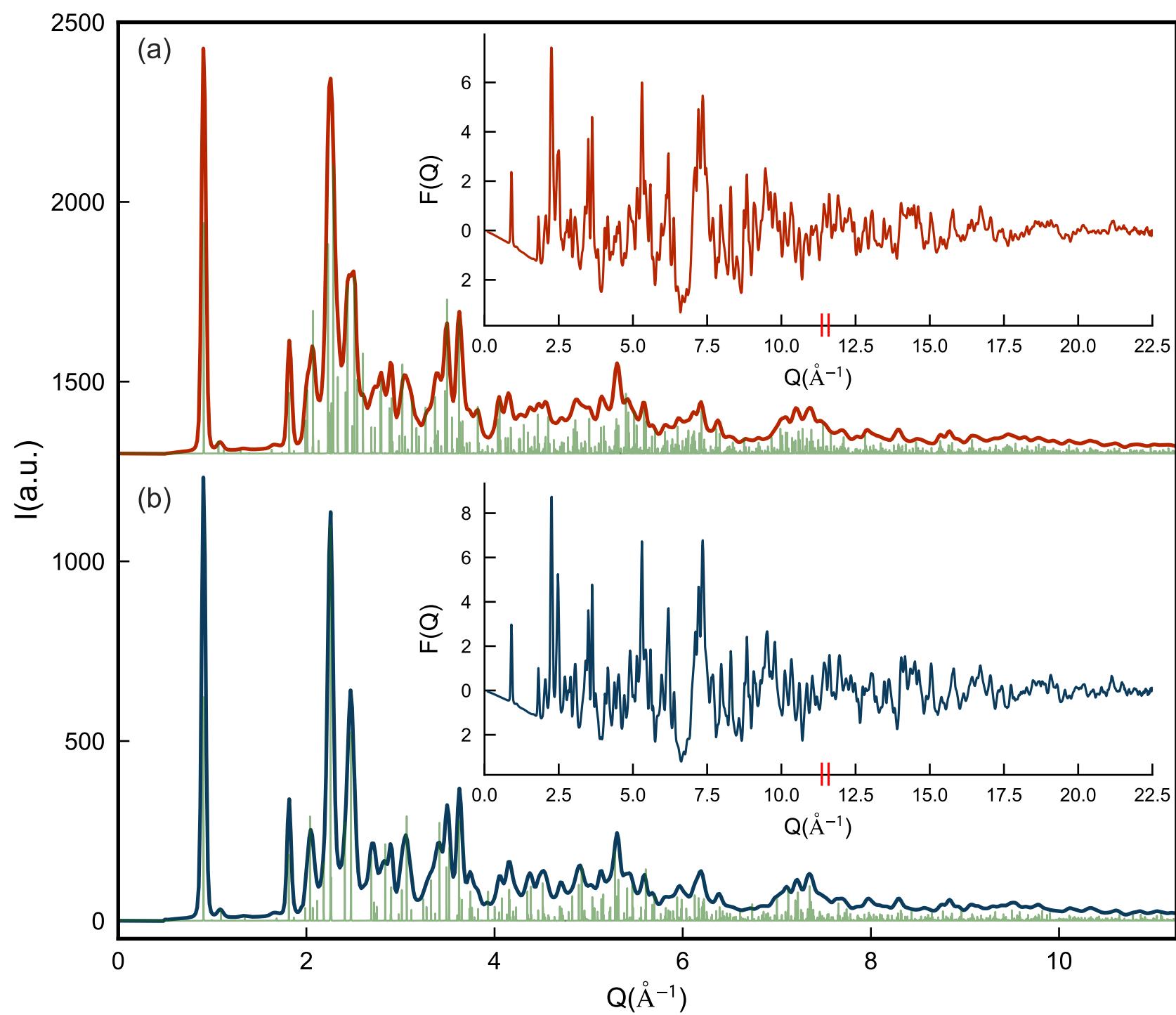


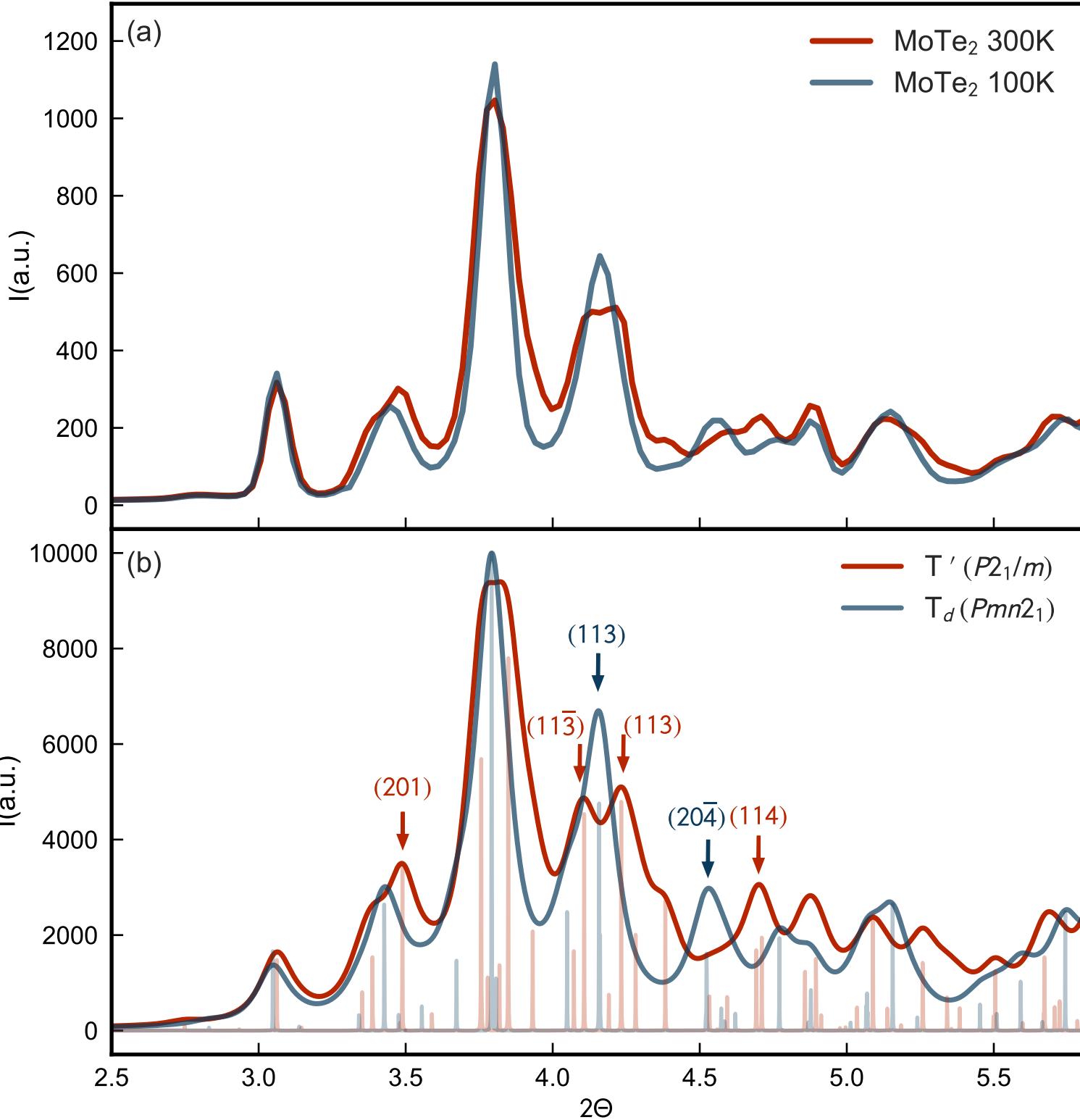


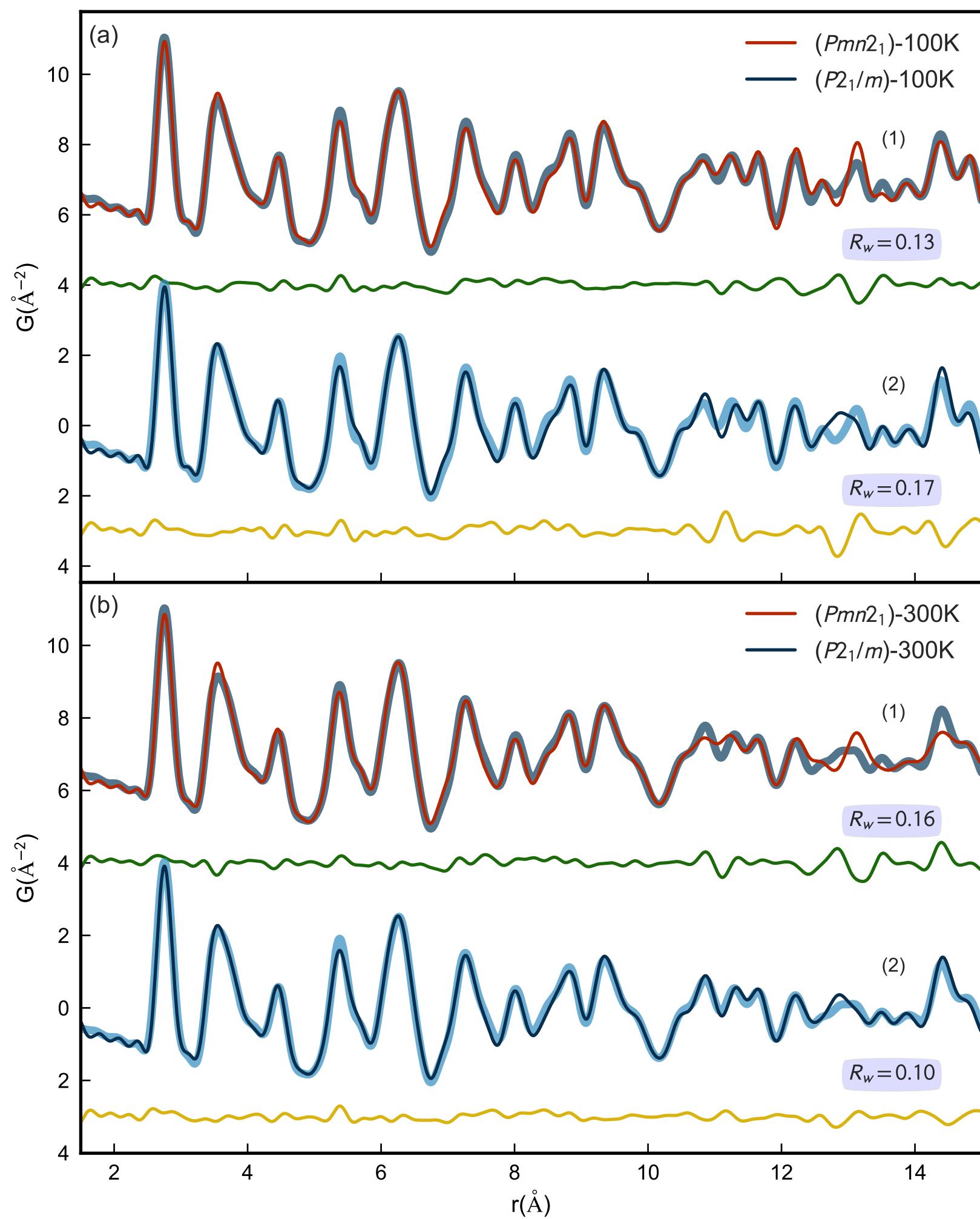


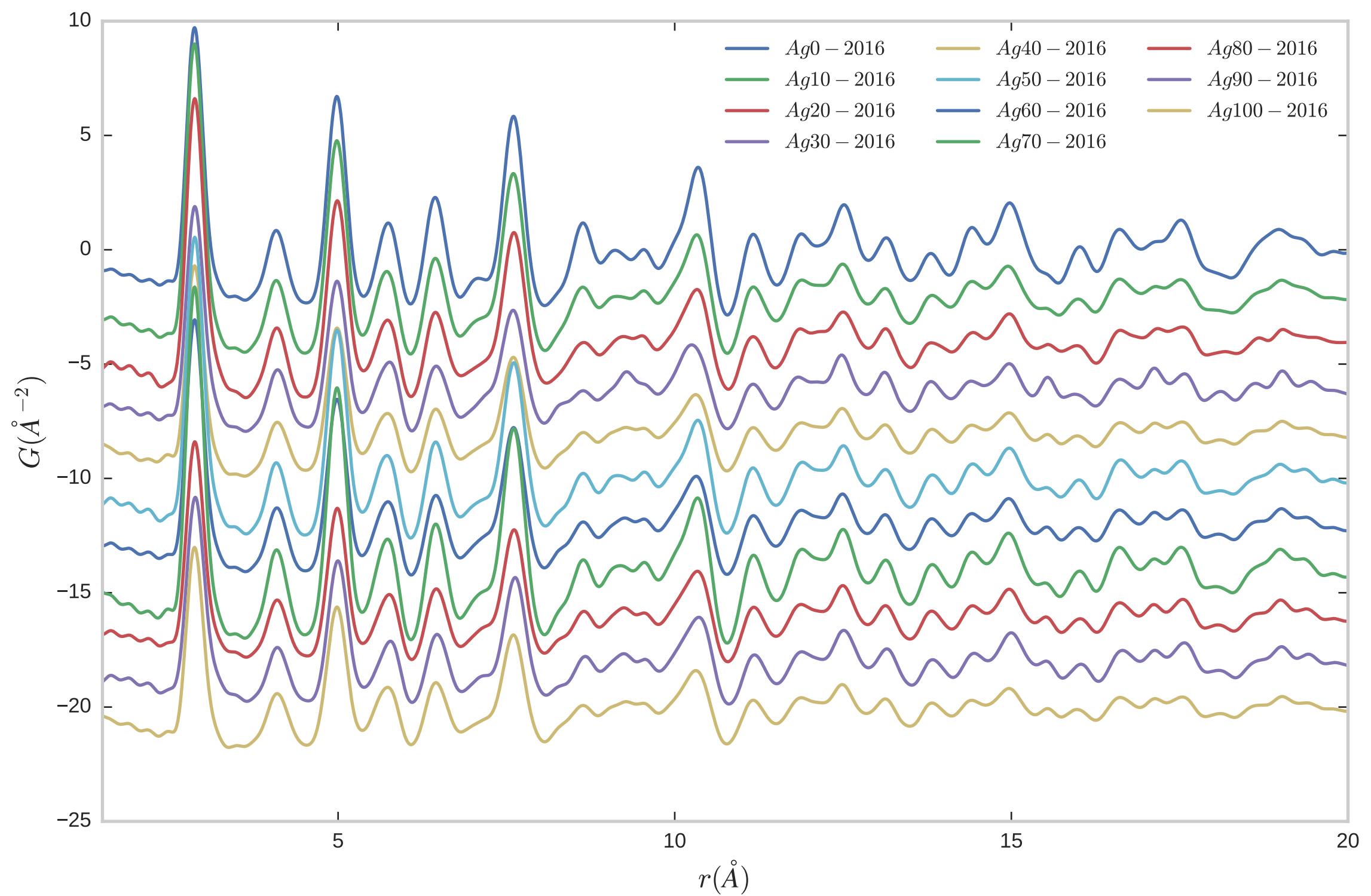


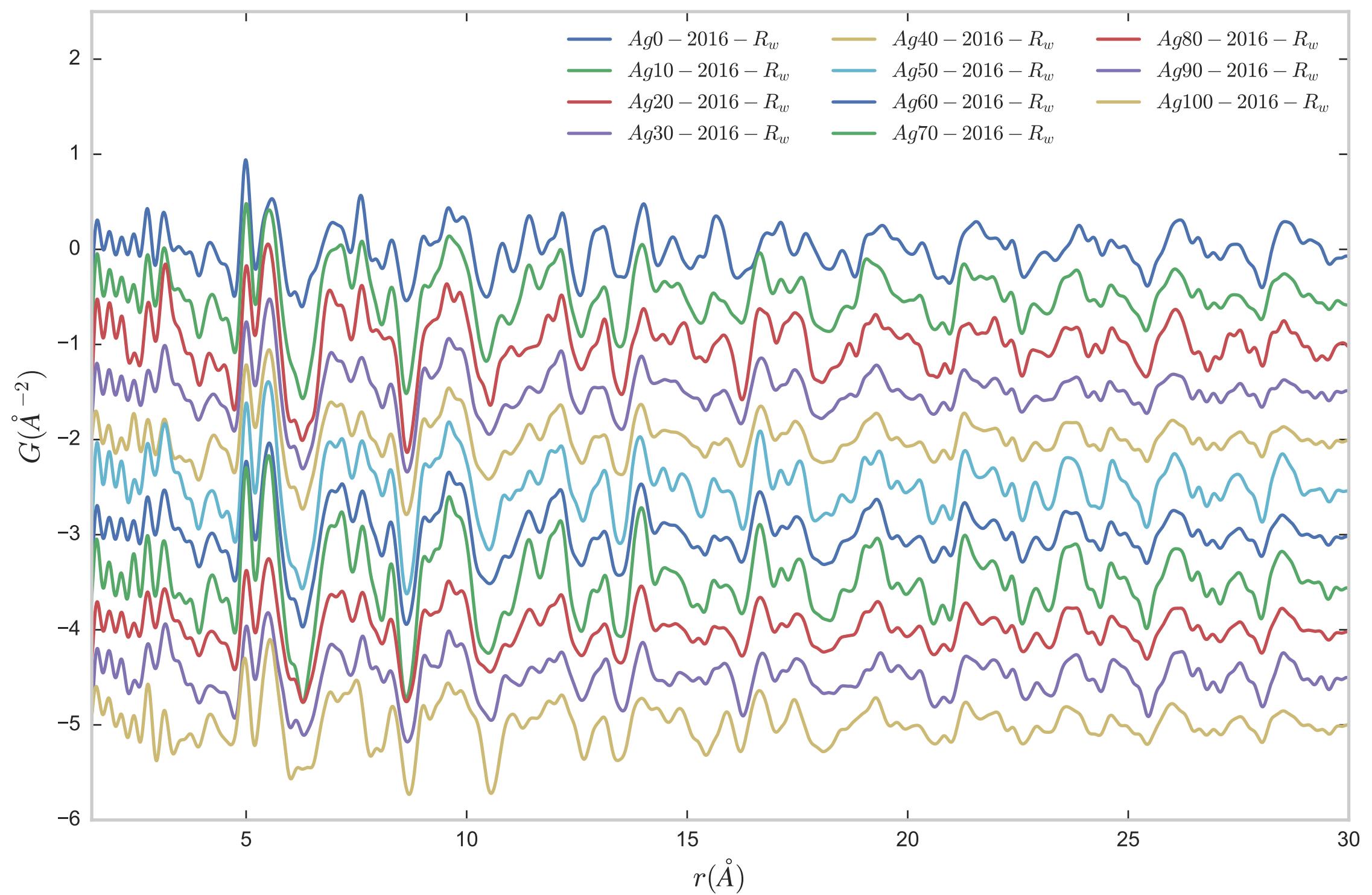


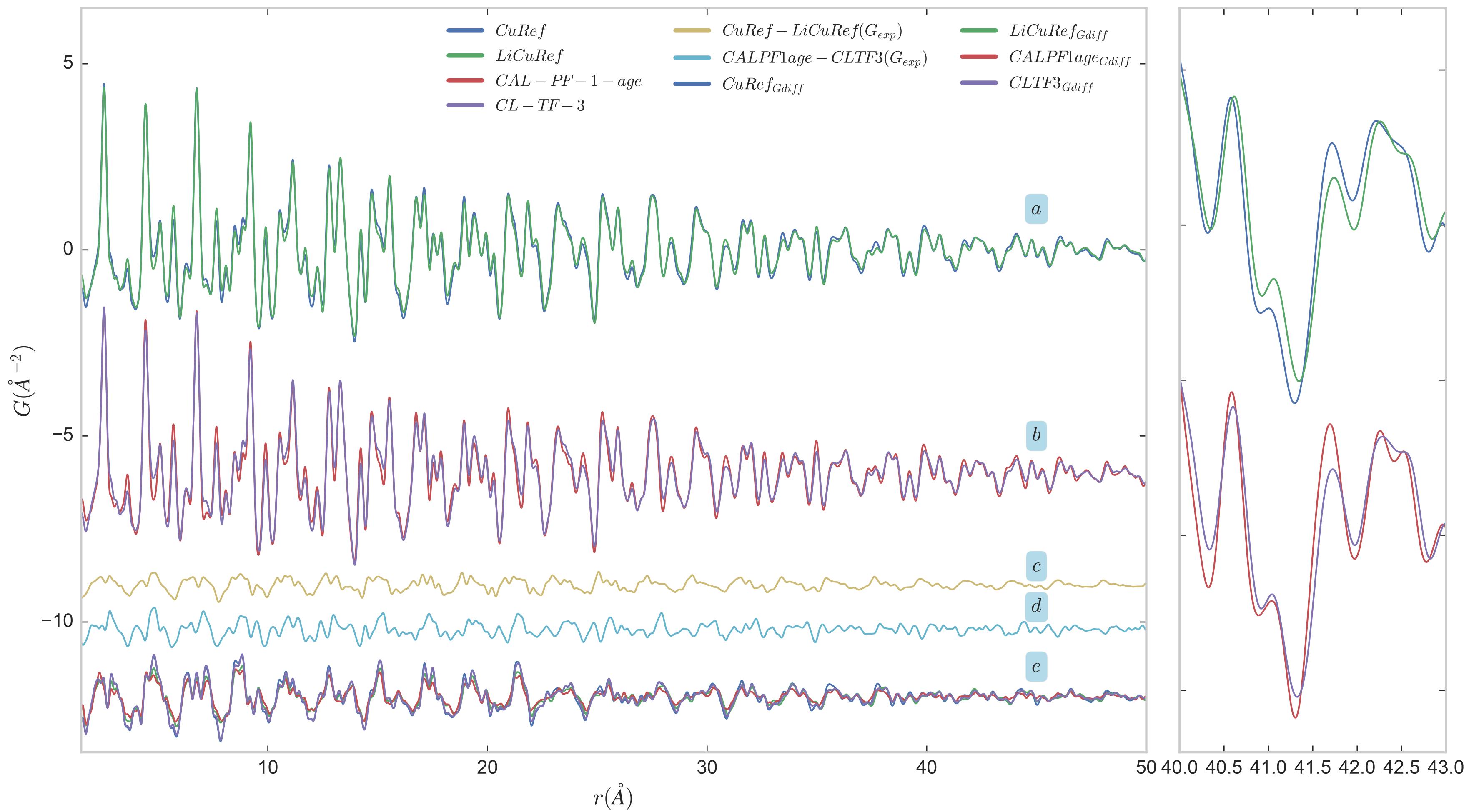


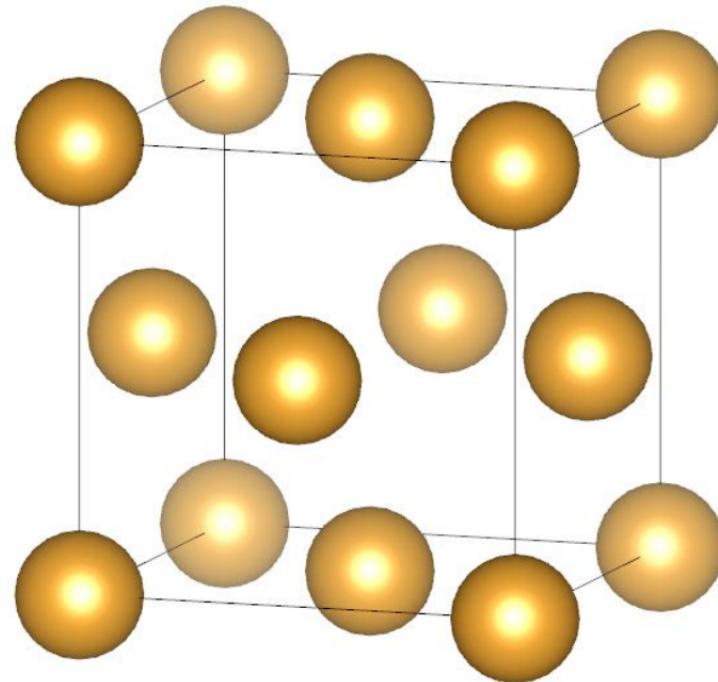




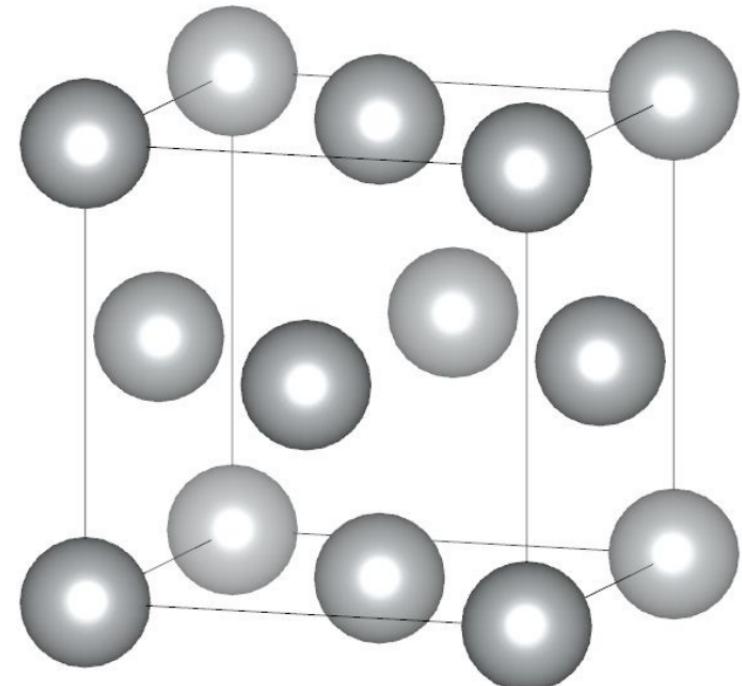
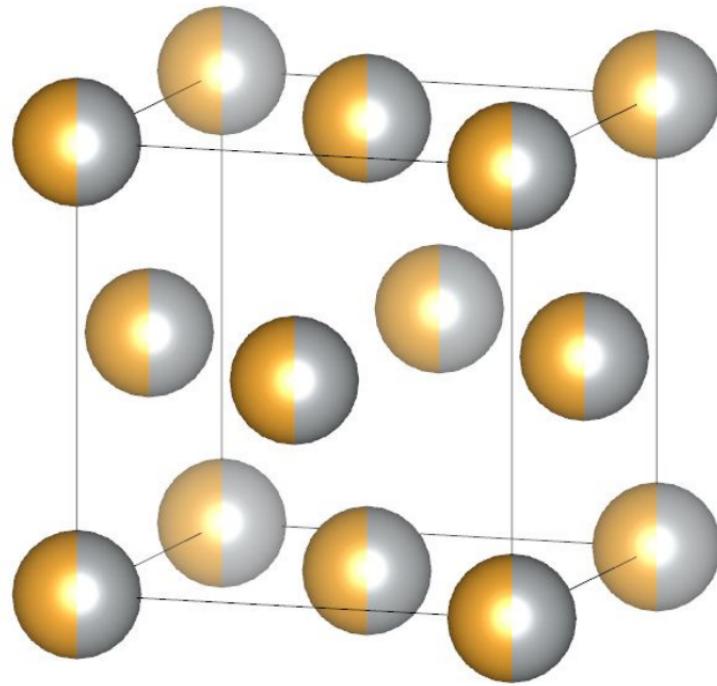




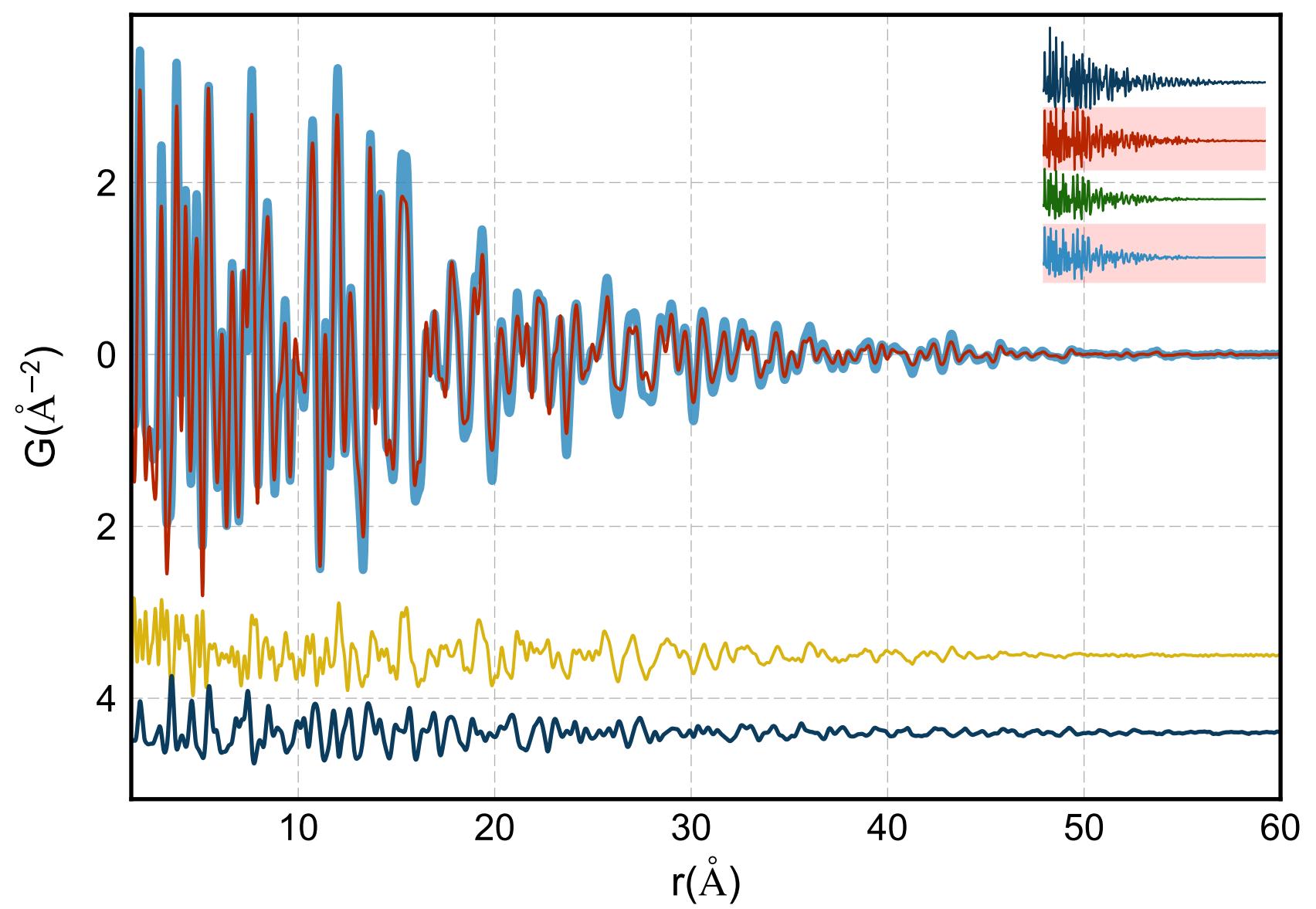


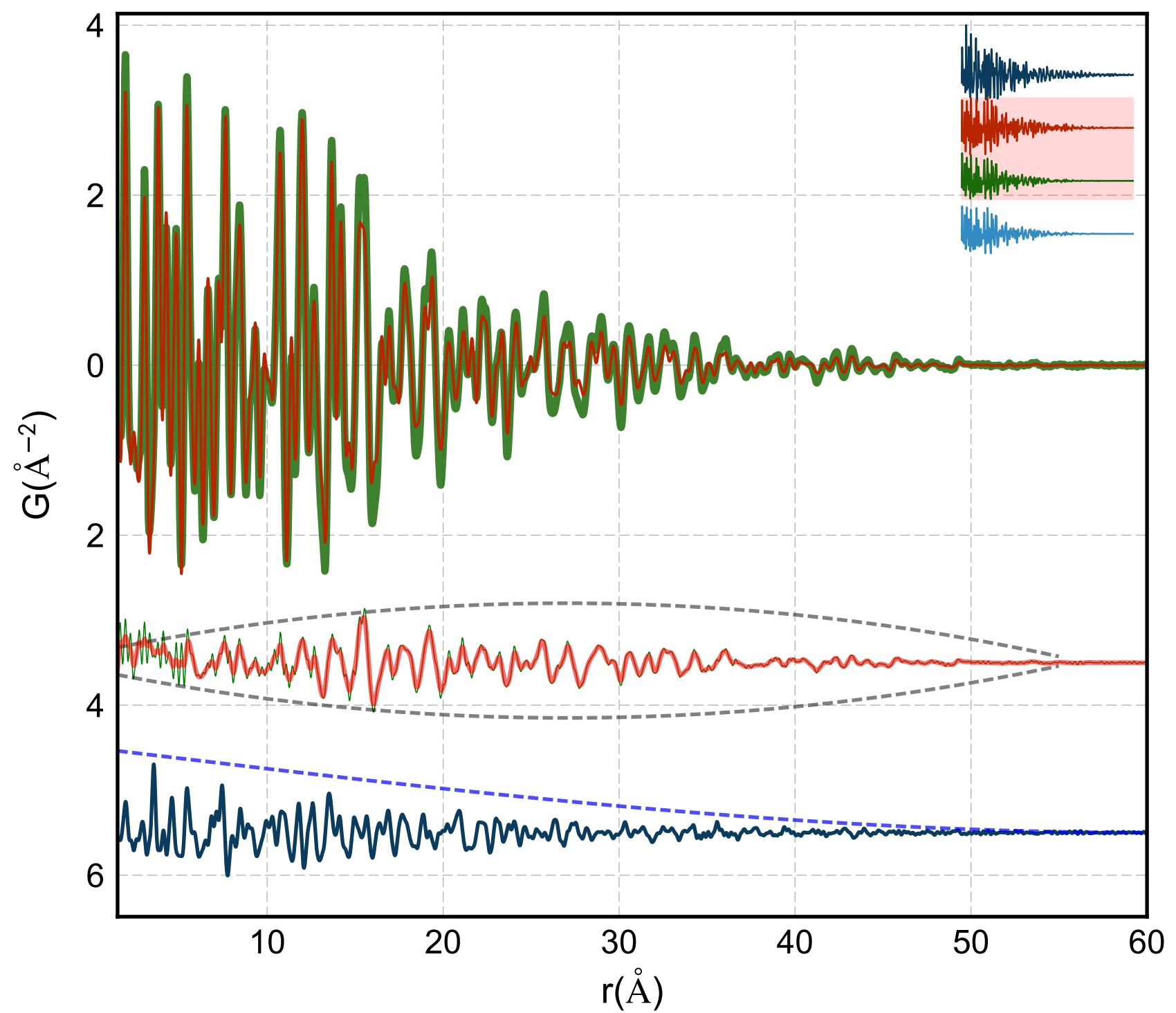


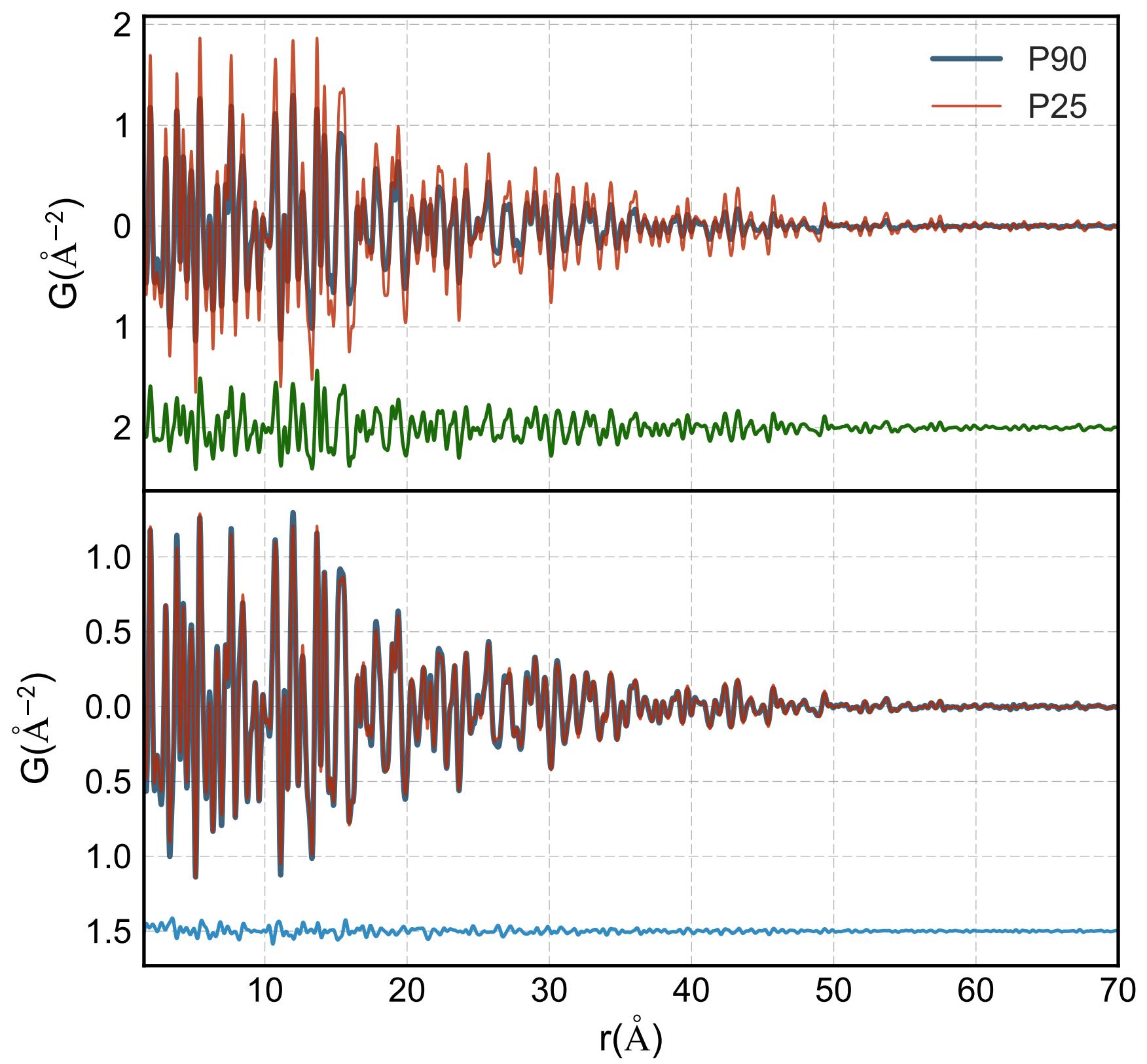
*Au*

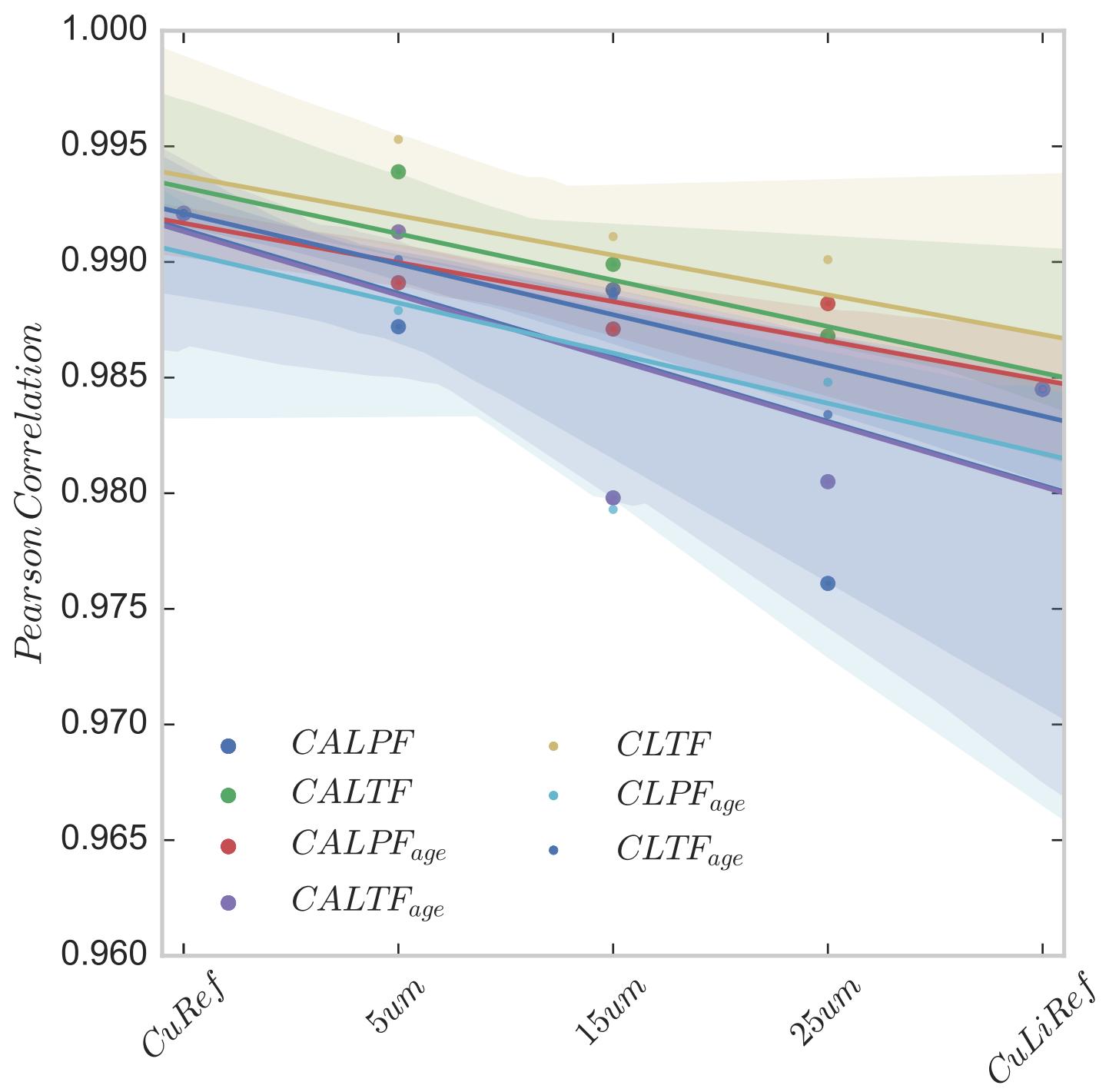


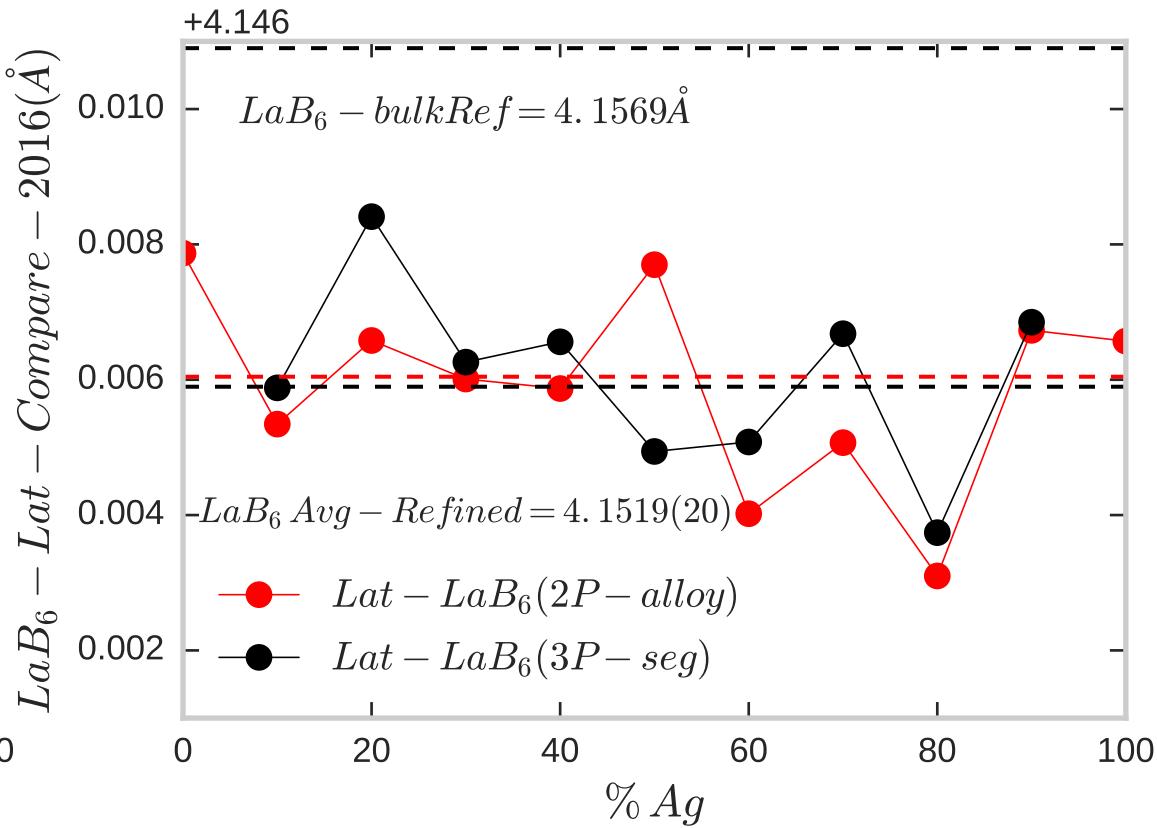
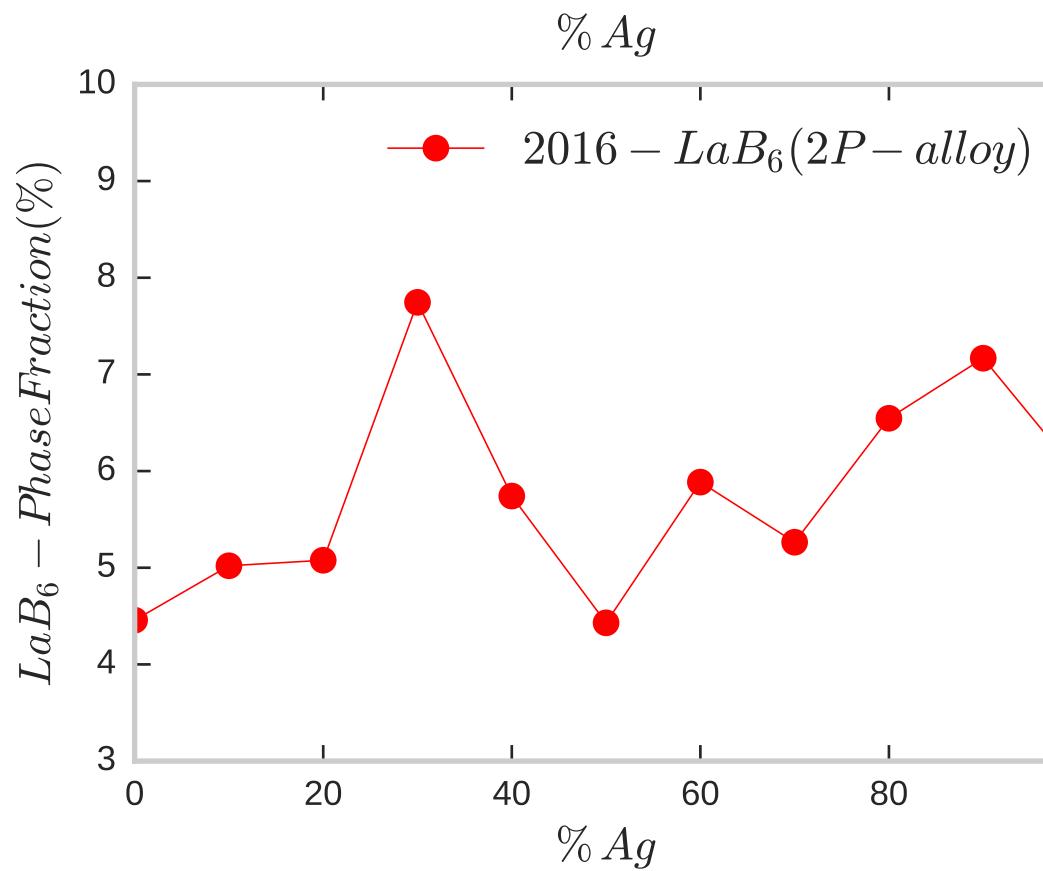
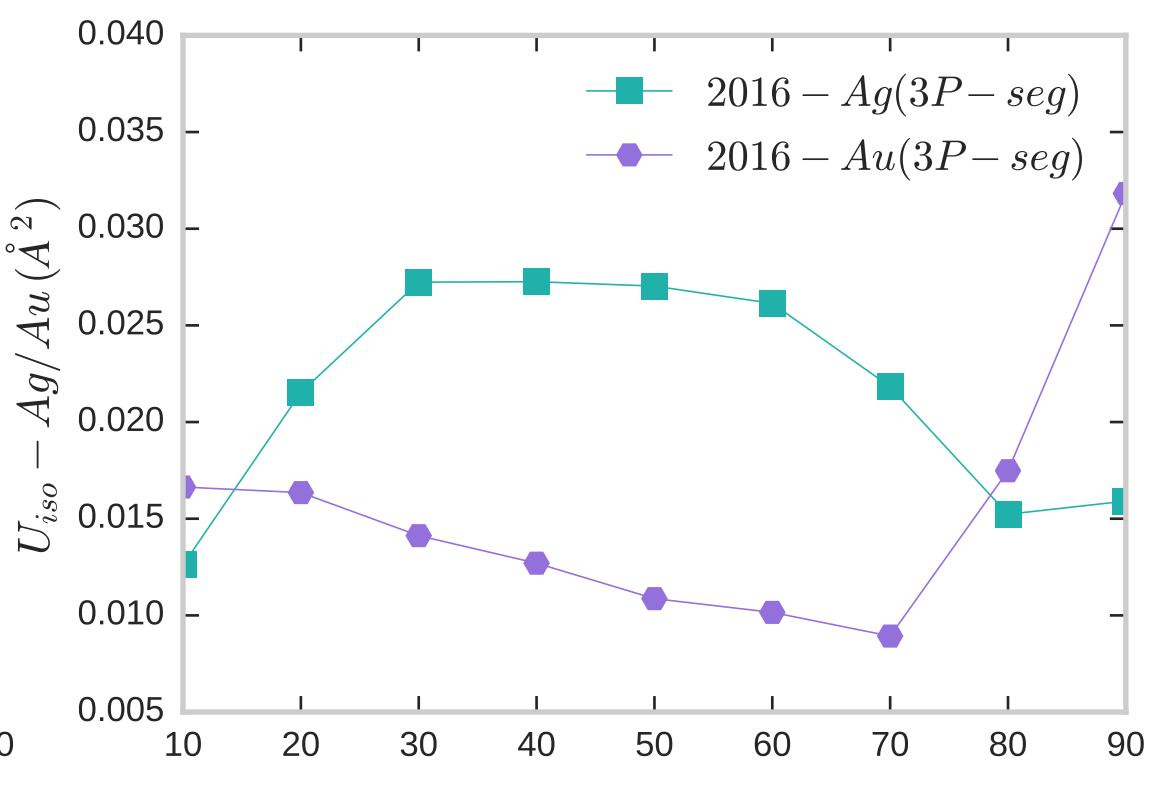
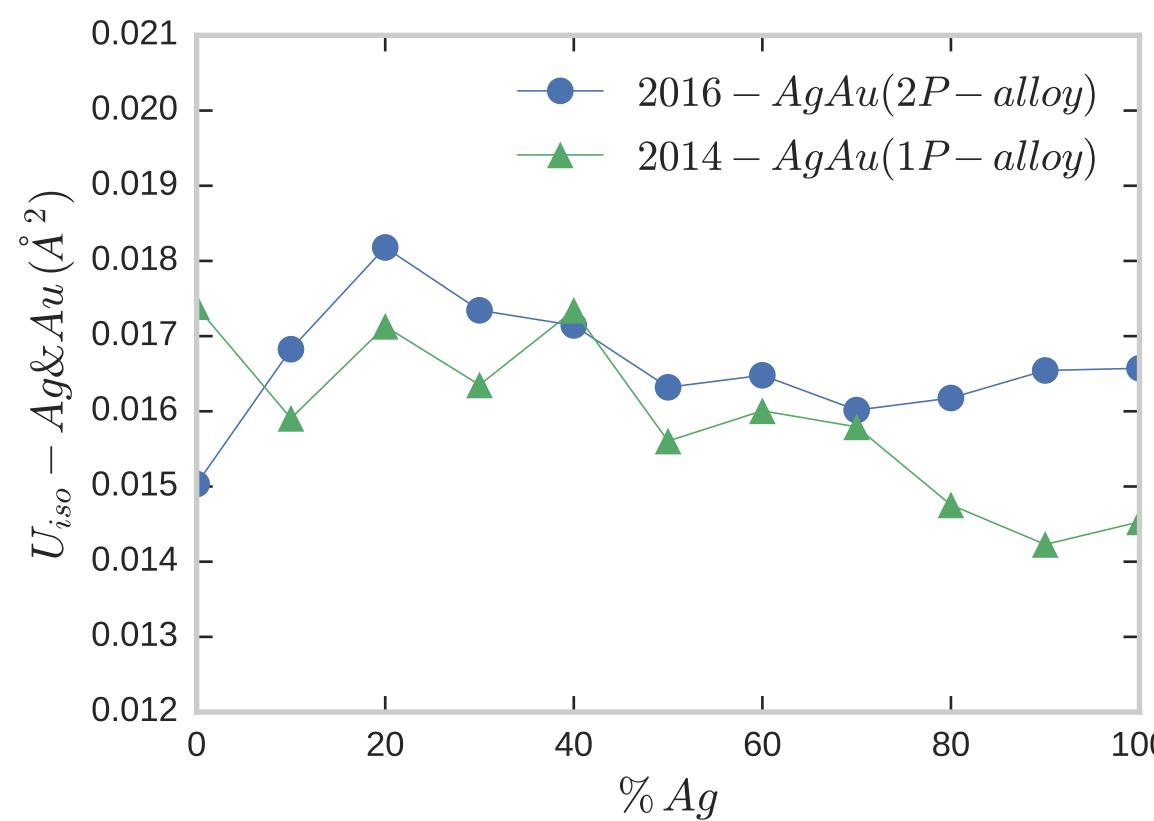
*Ag*

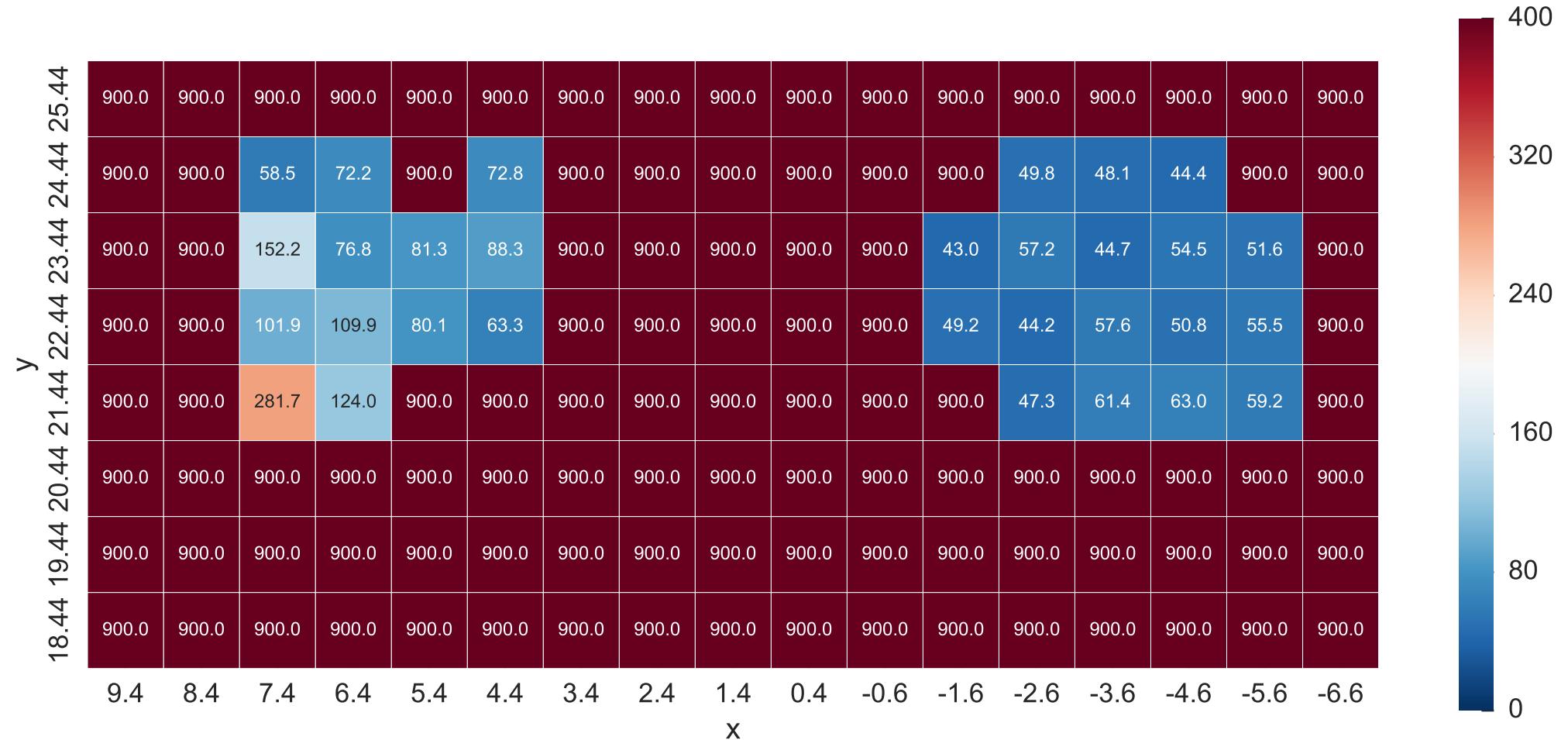


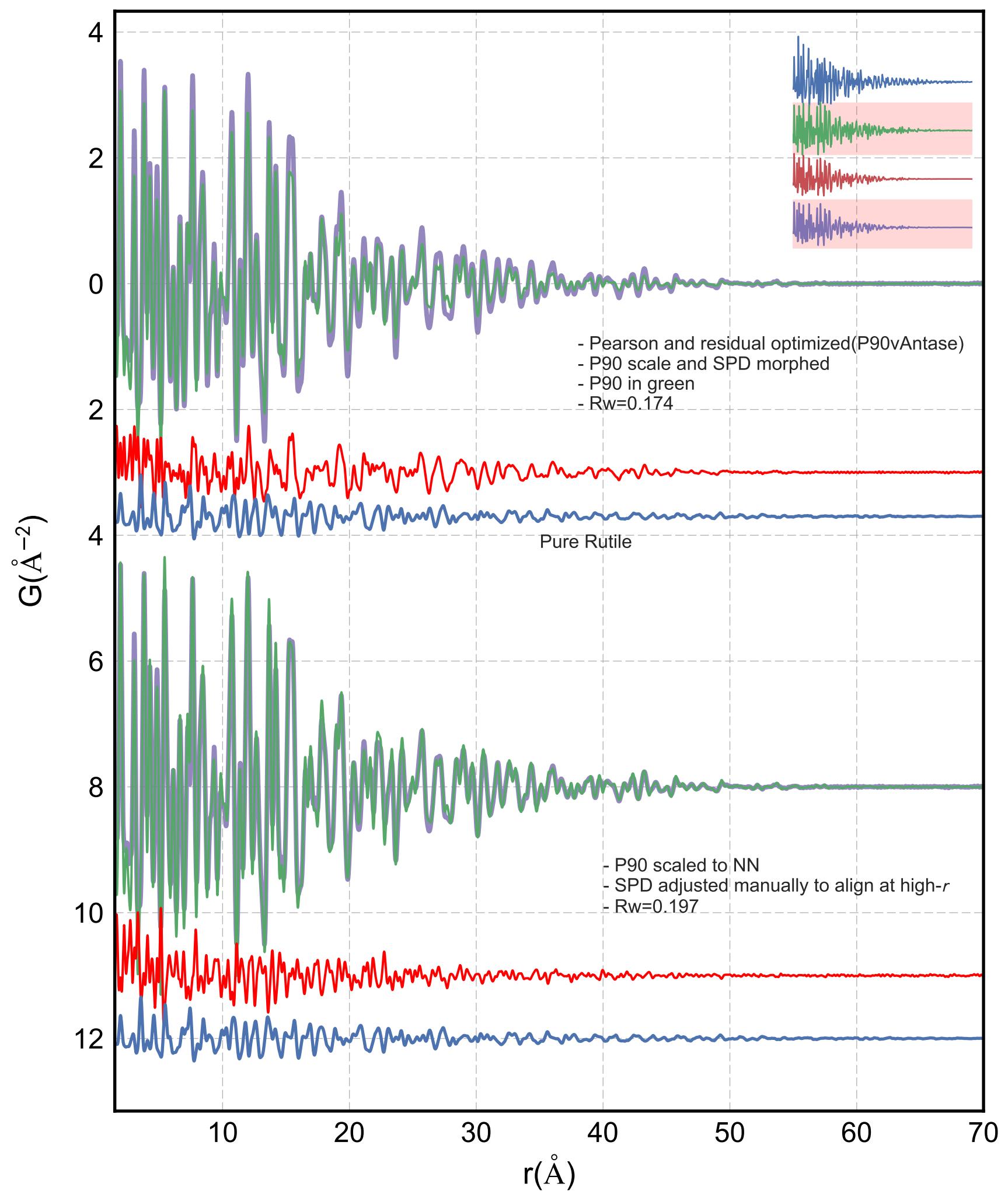


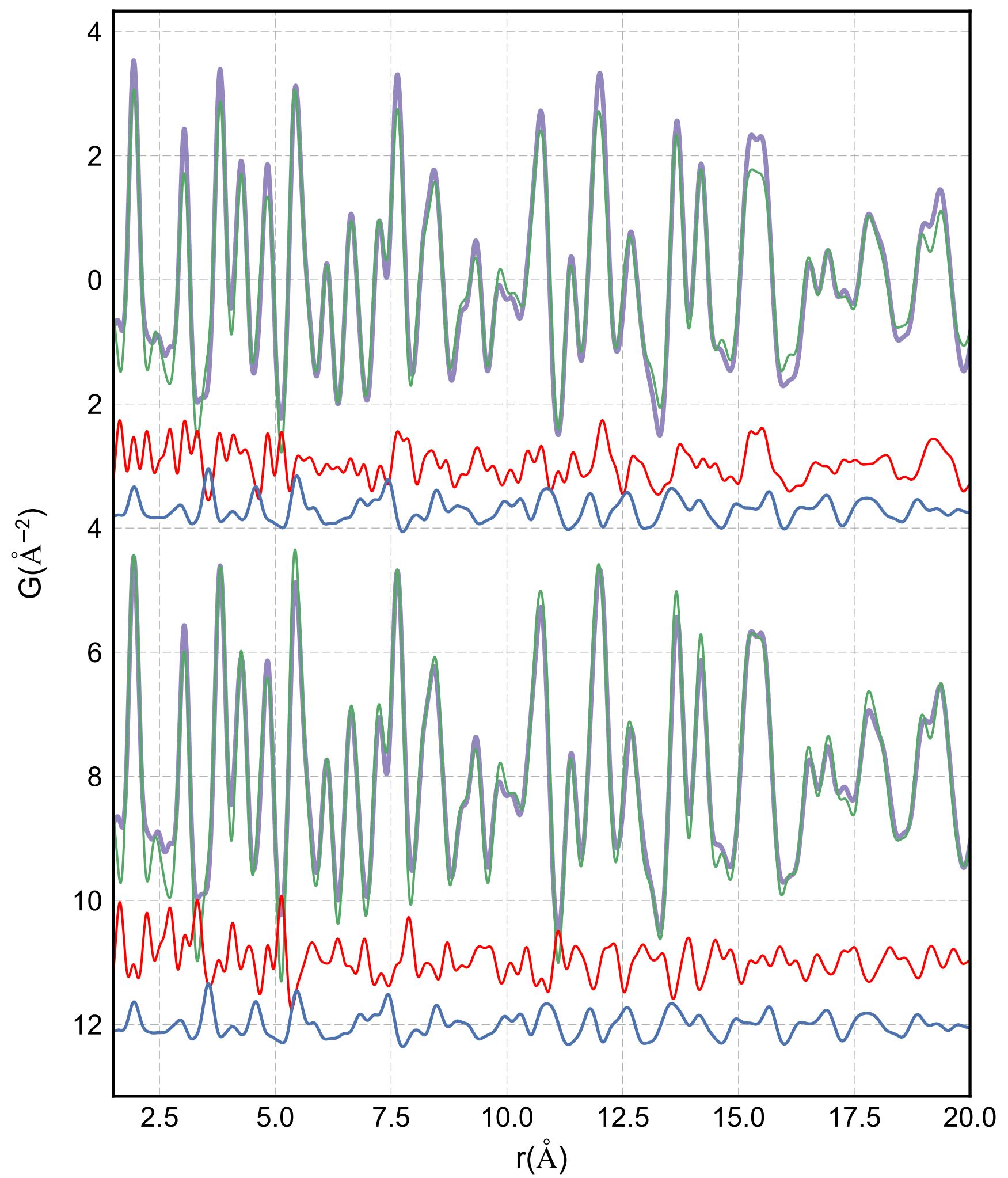


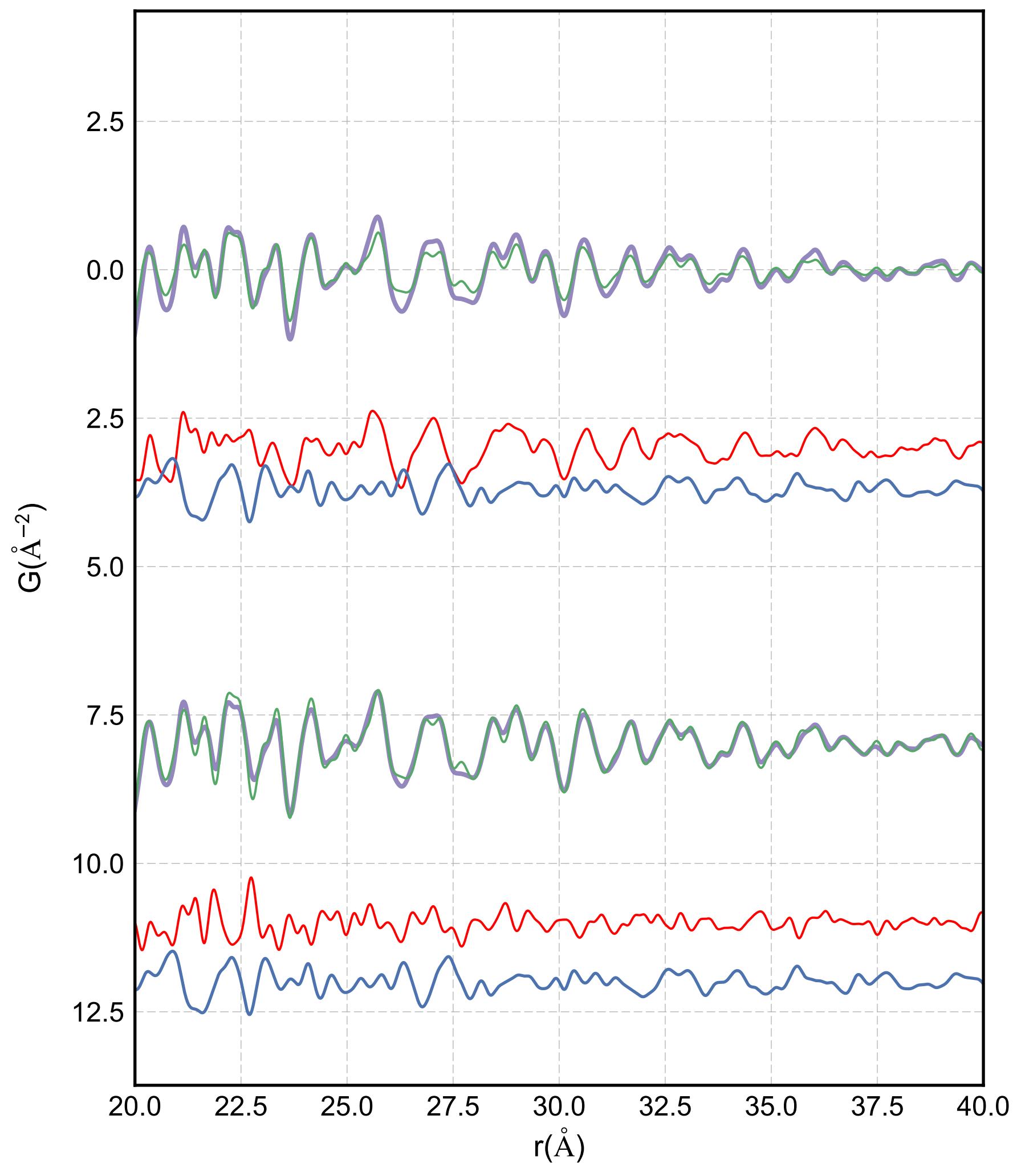


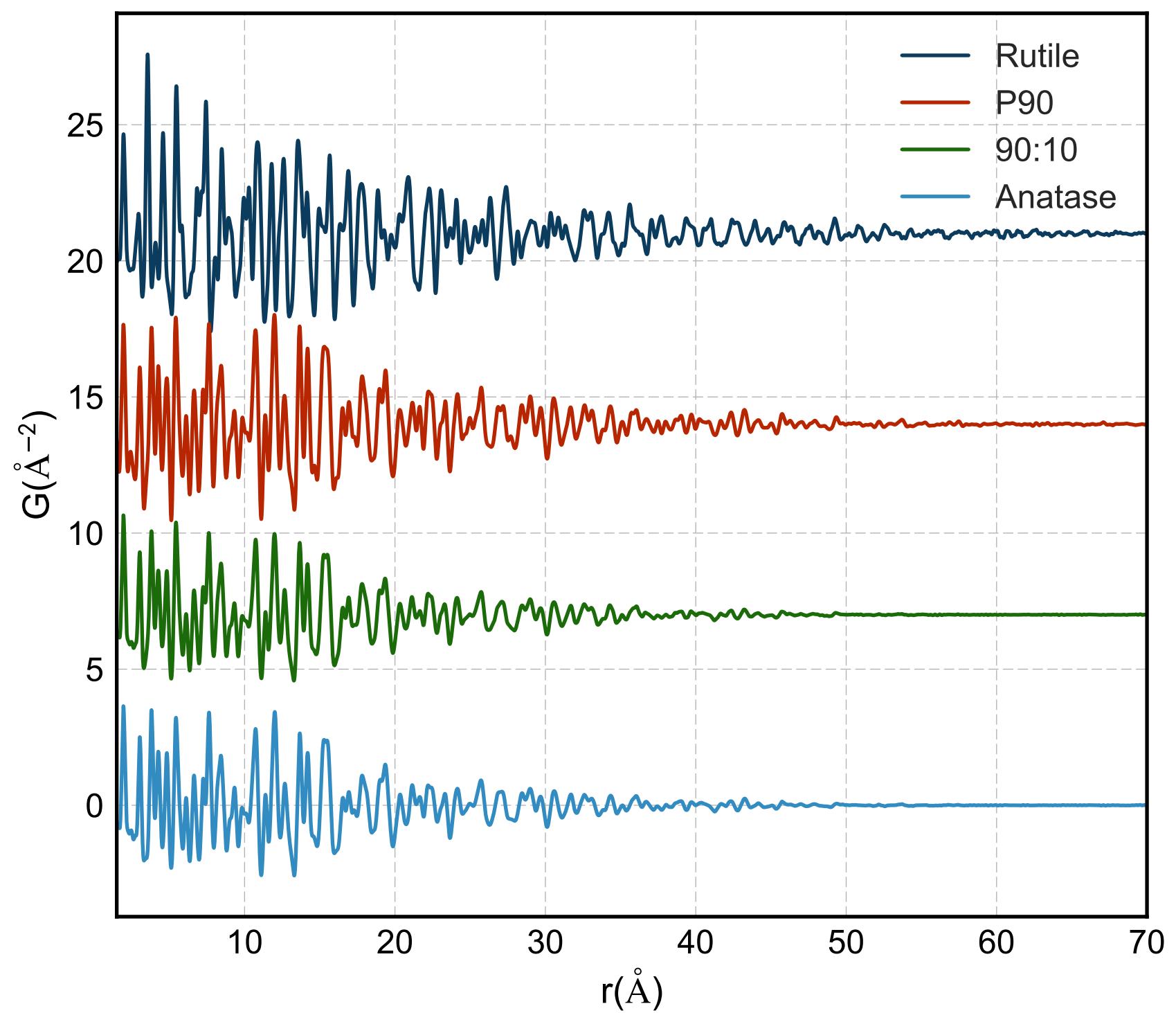


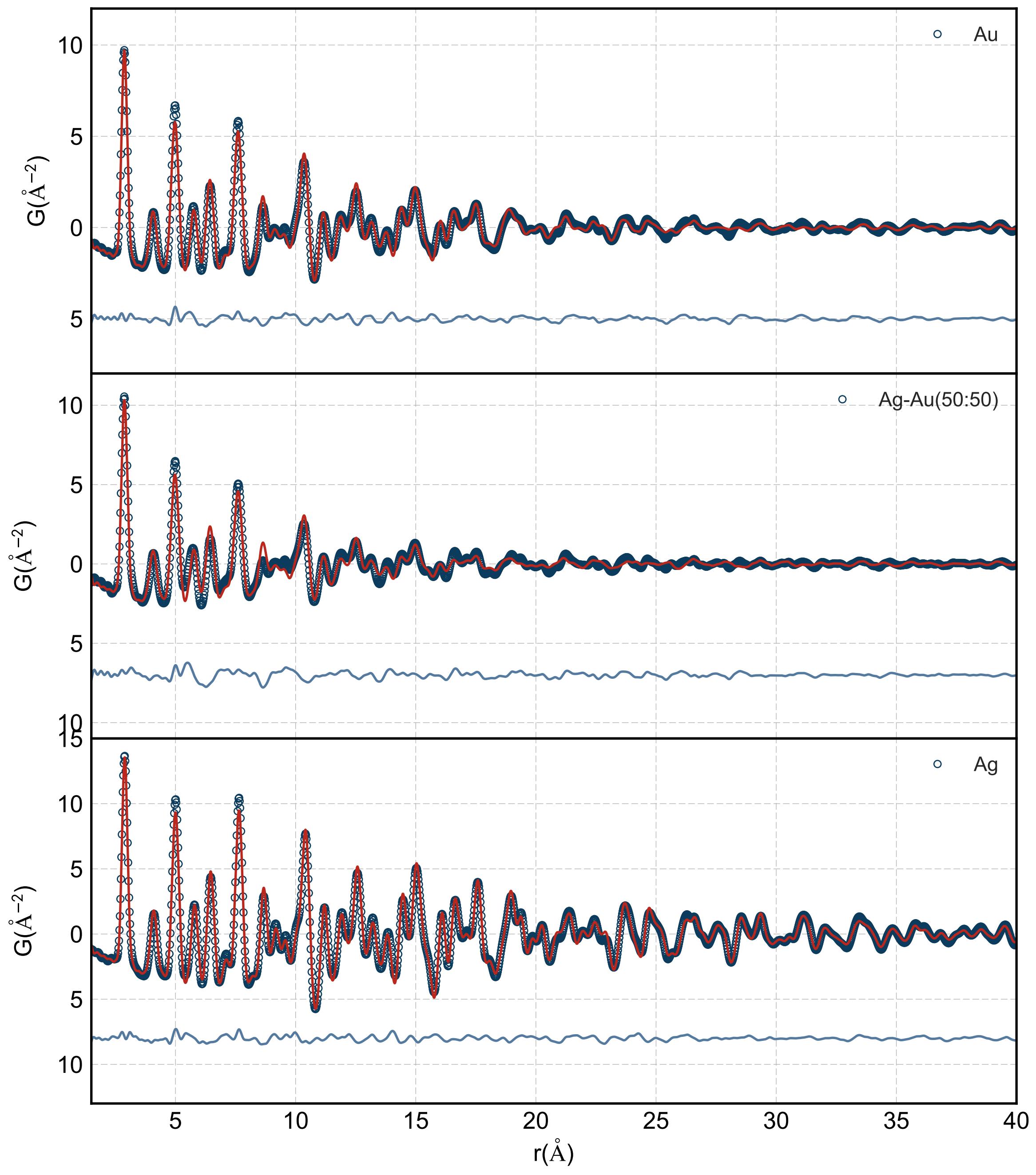


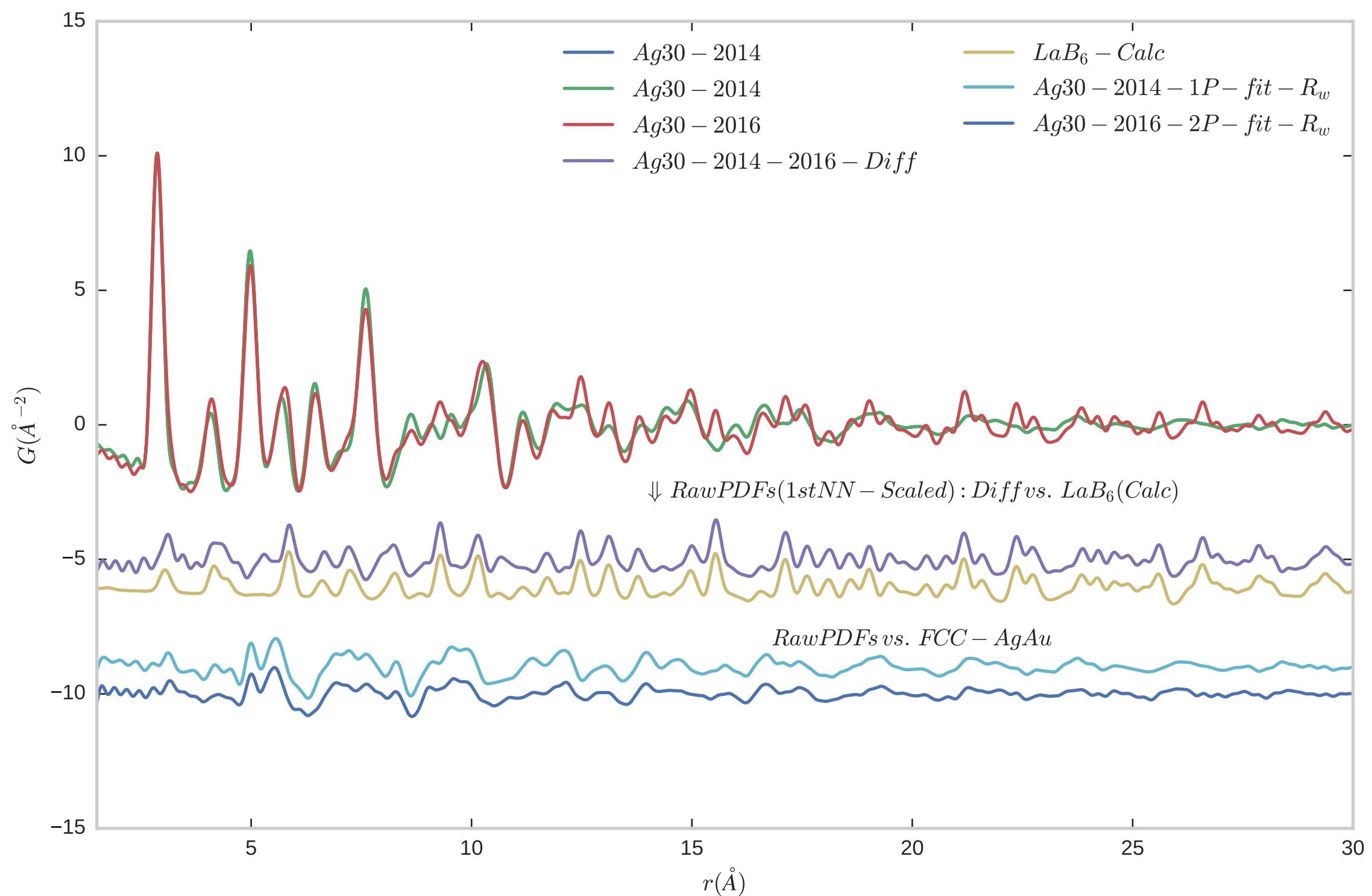






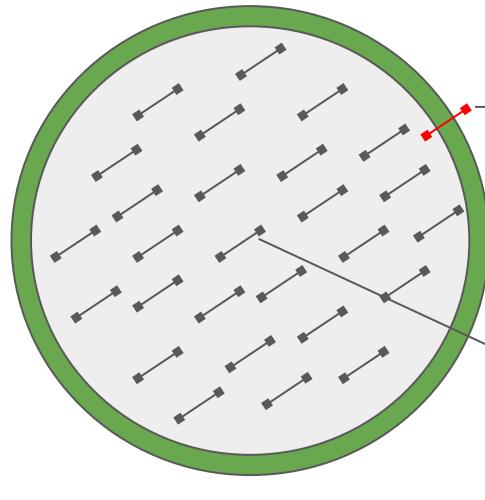








CS-Model (low-R)



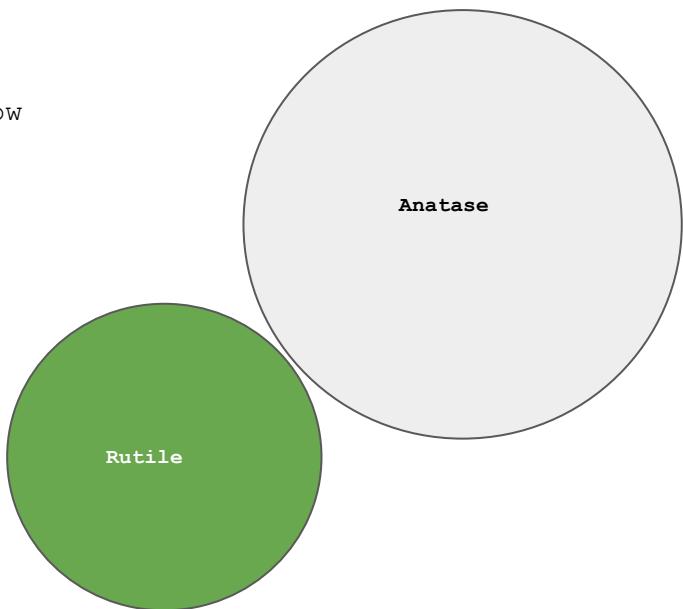
P-size: >25nm

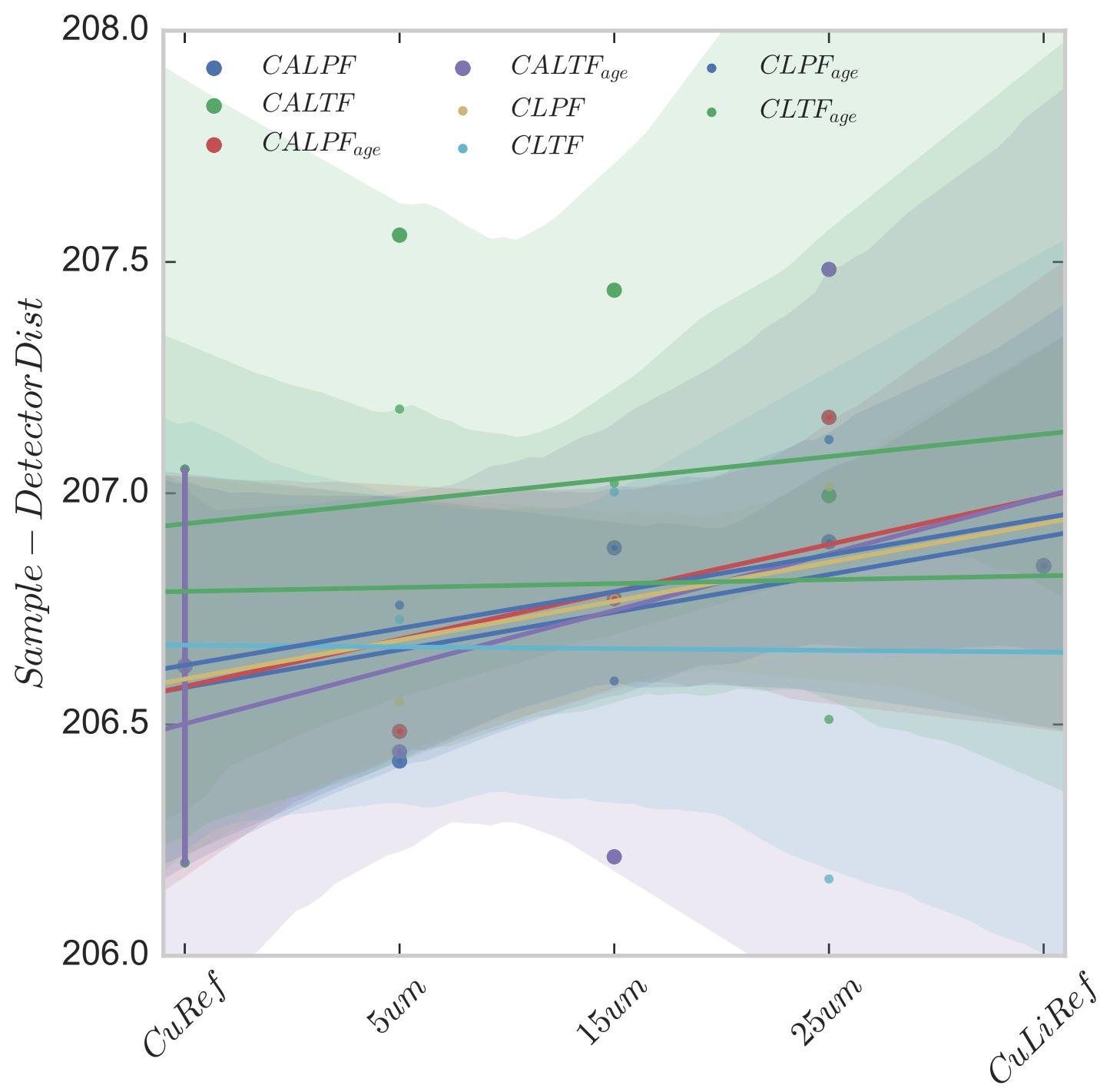
WAXS resolution: ~7-8nm

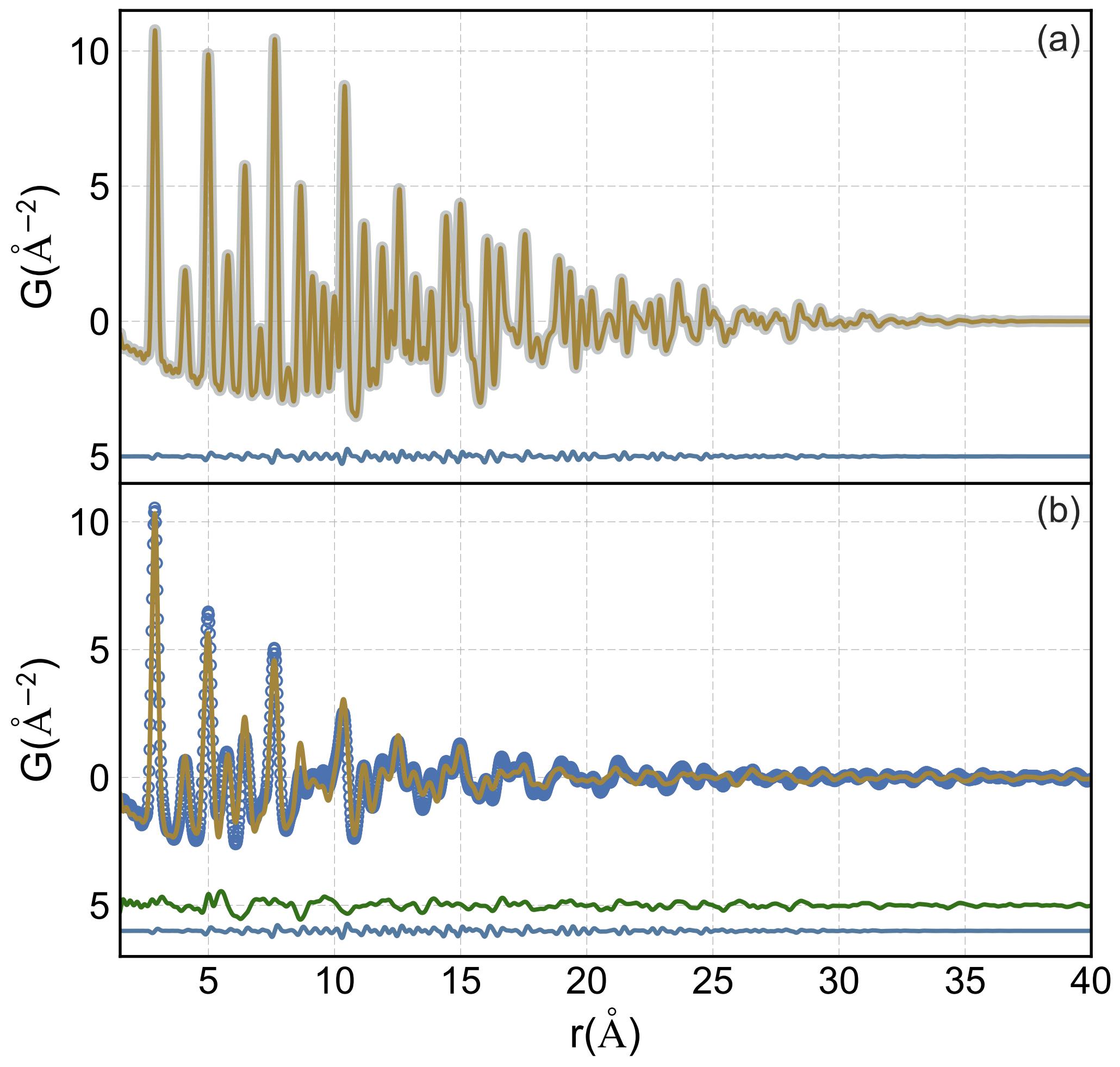
Rutile Correlations (low-R, low probability/phase %, reduced coherence)

Anatase Correlations (low-R, high probability/phase %, LRO coherence)

Poly-Model







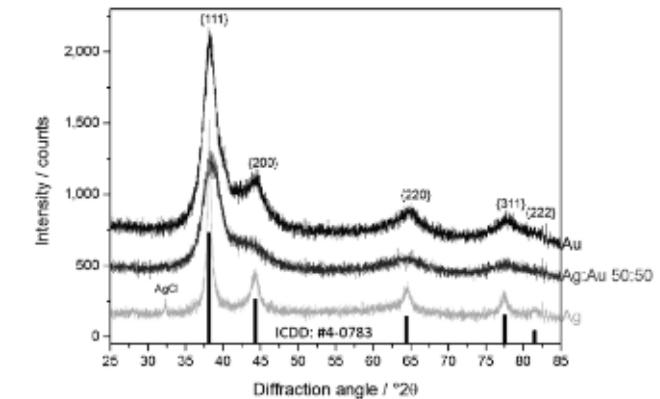
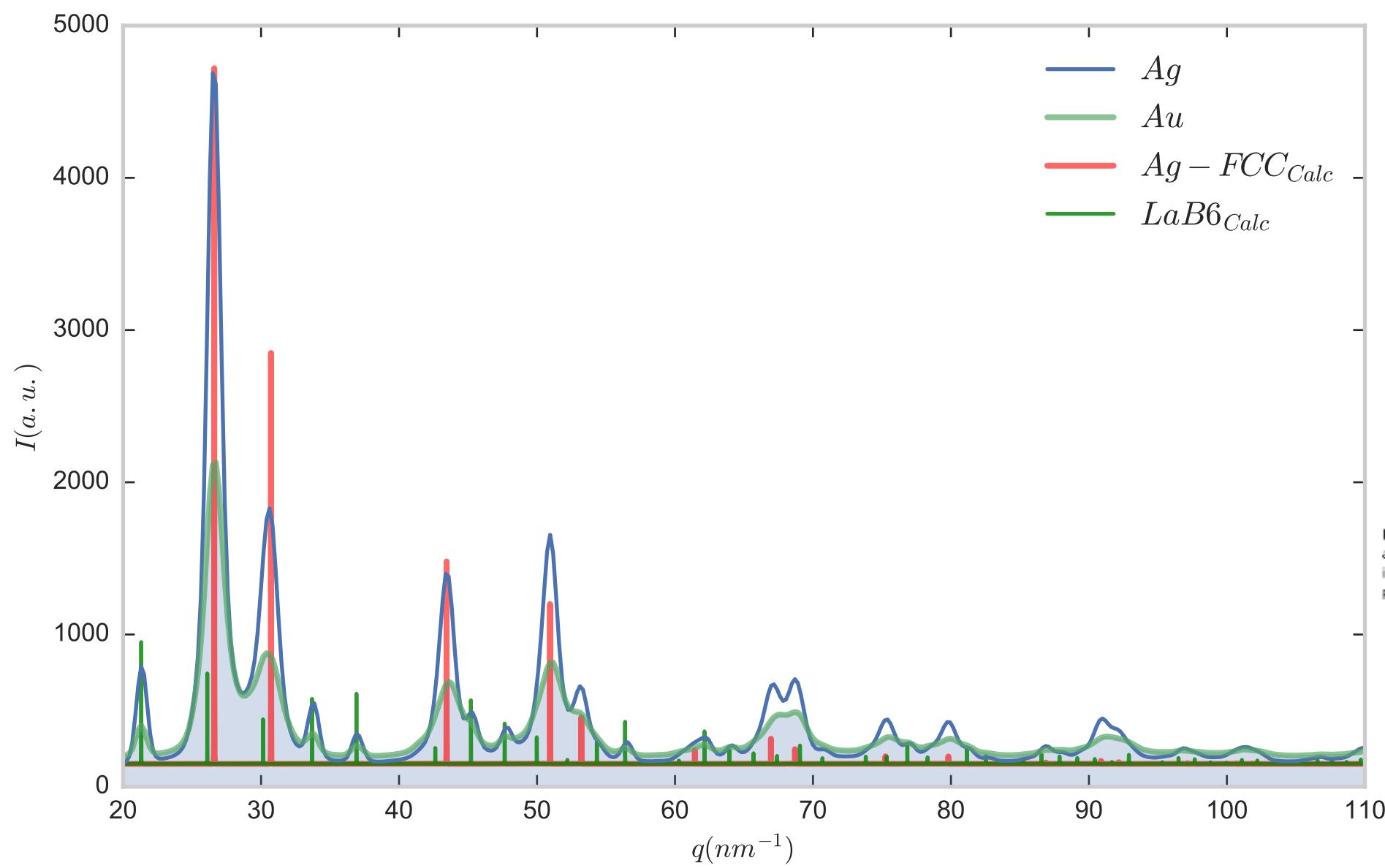
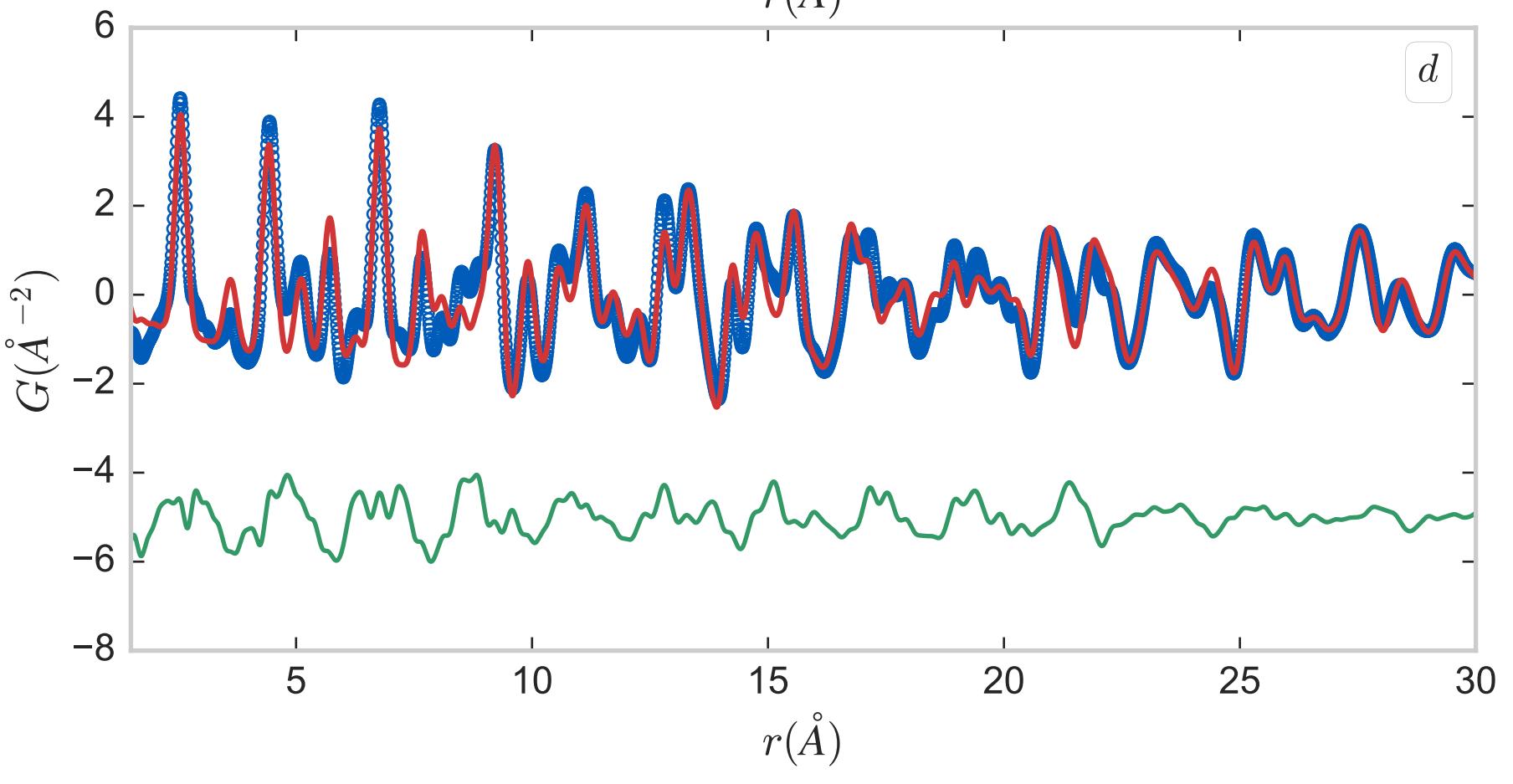
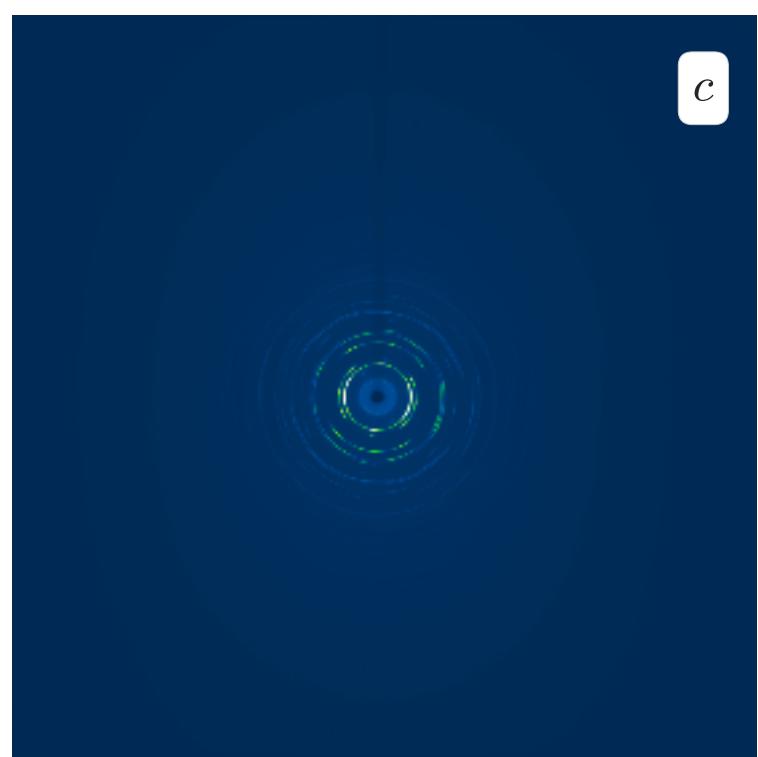
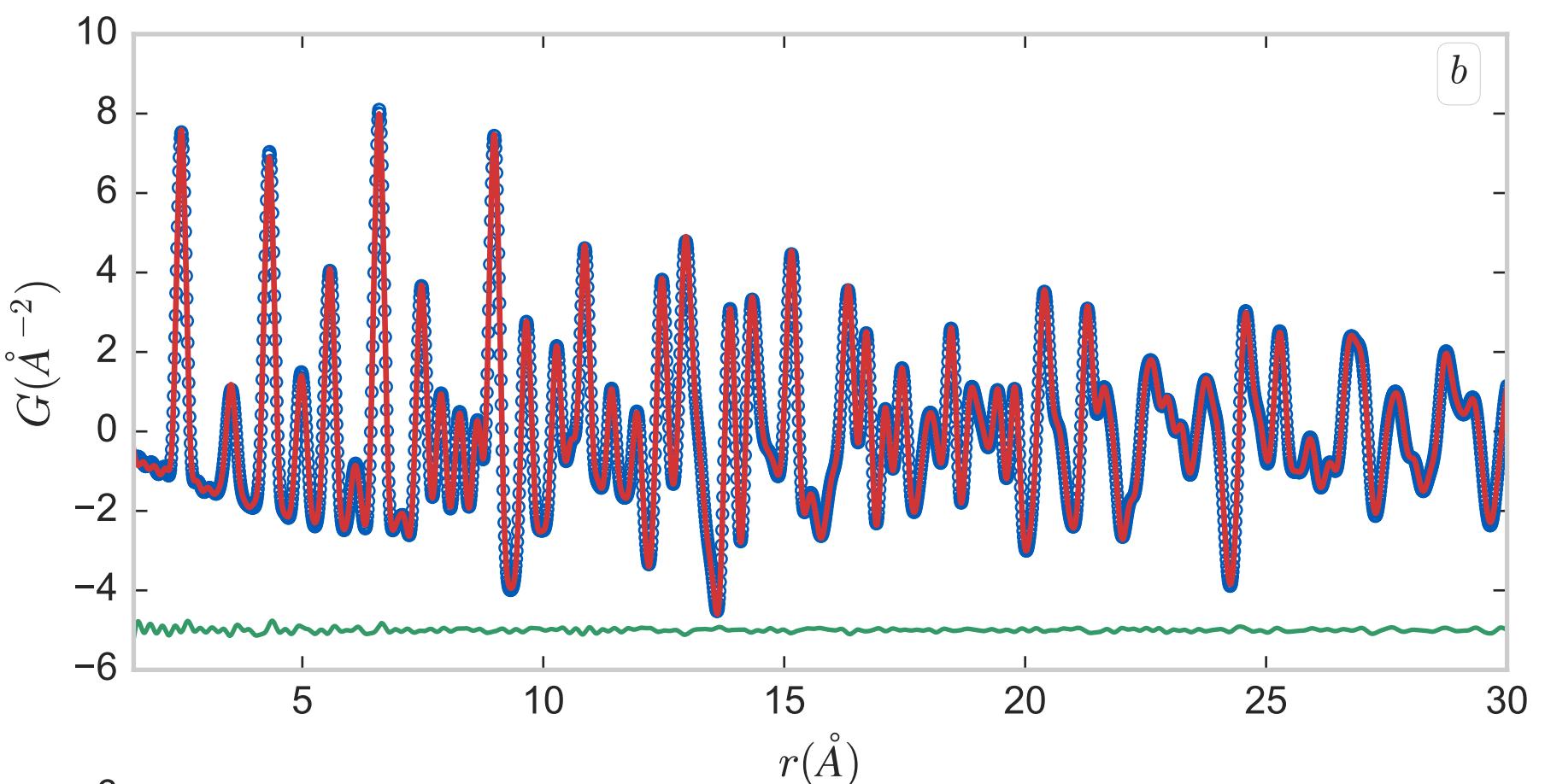
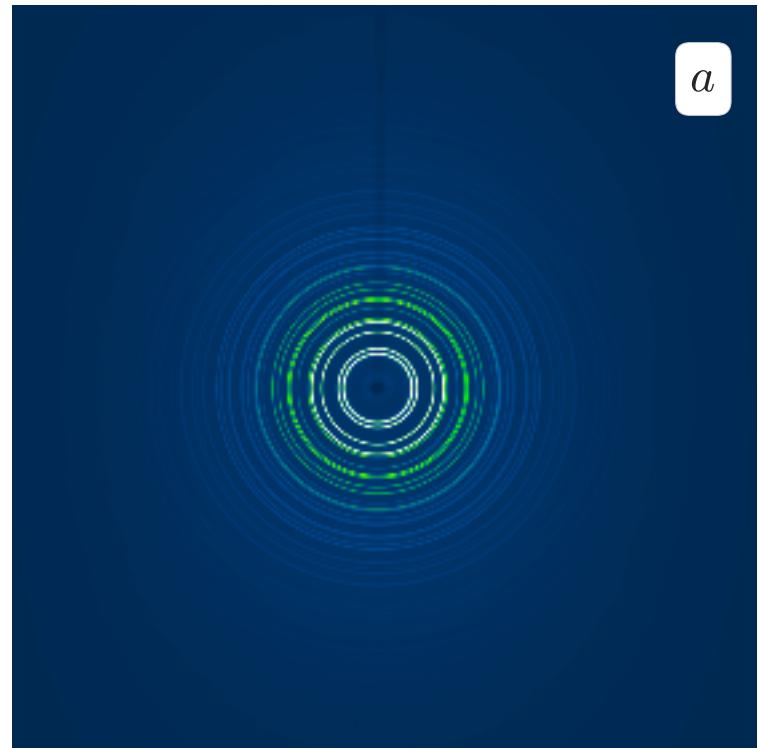
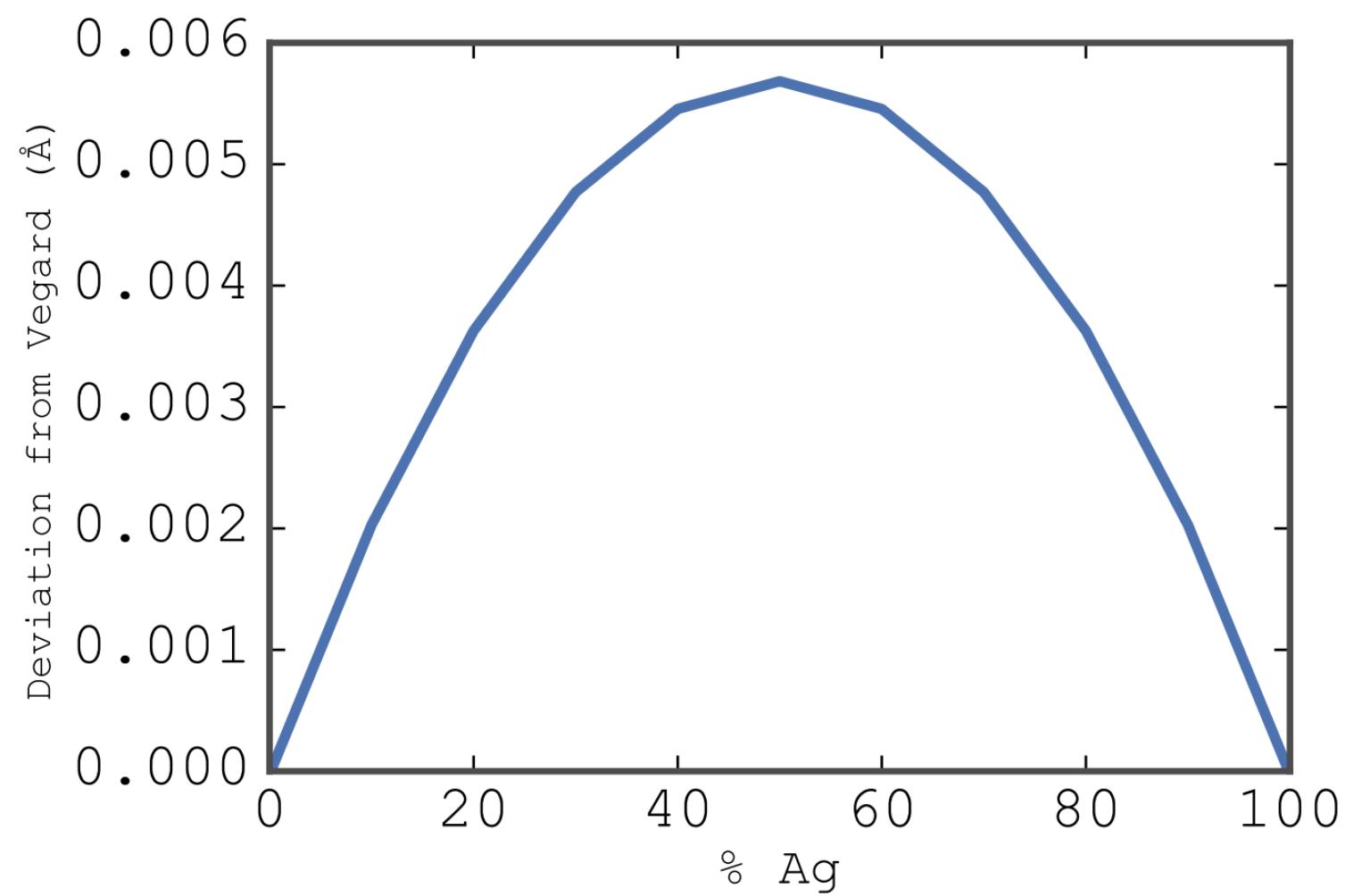
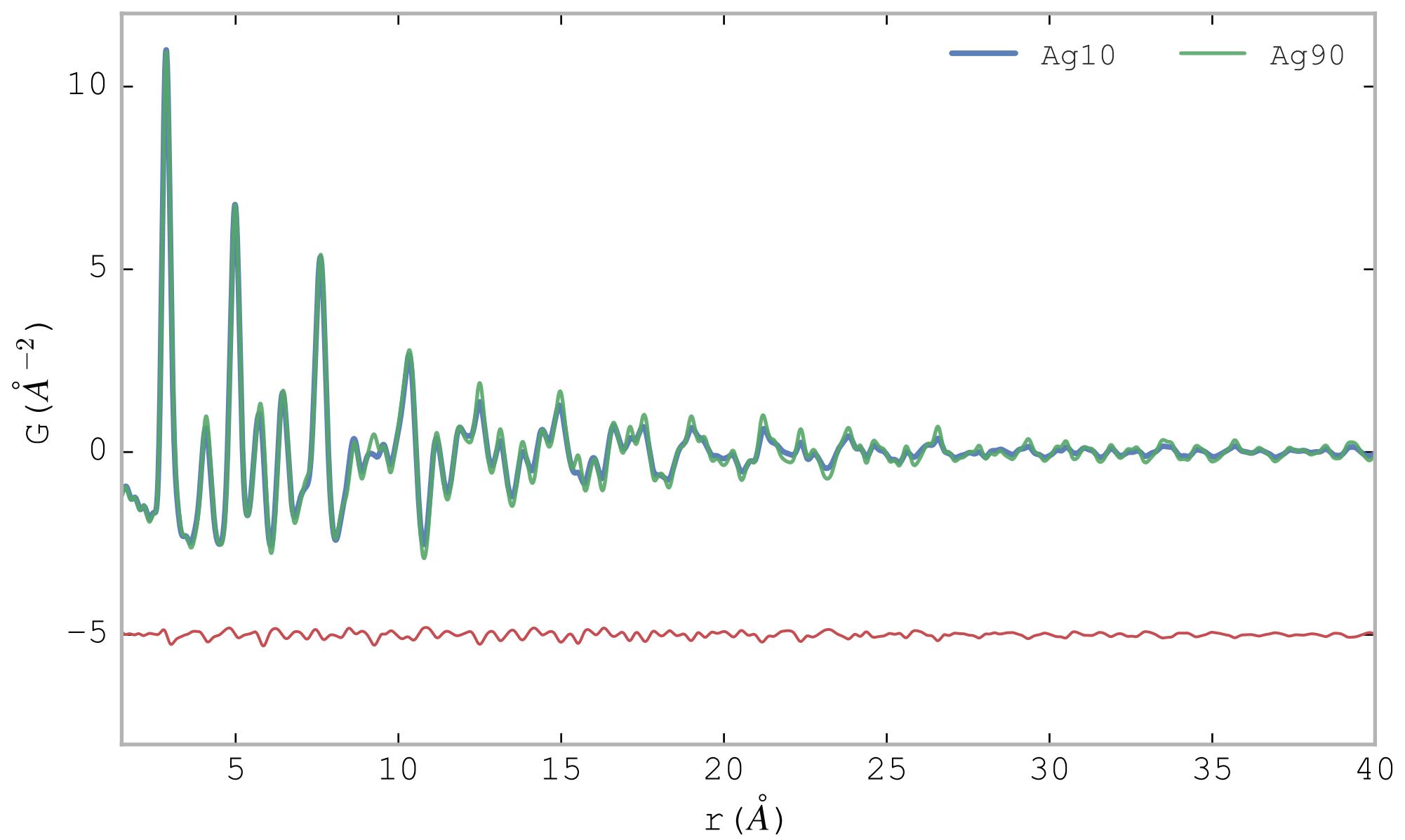
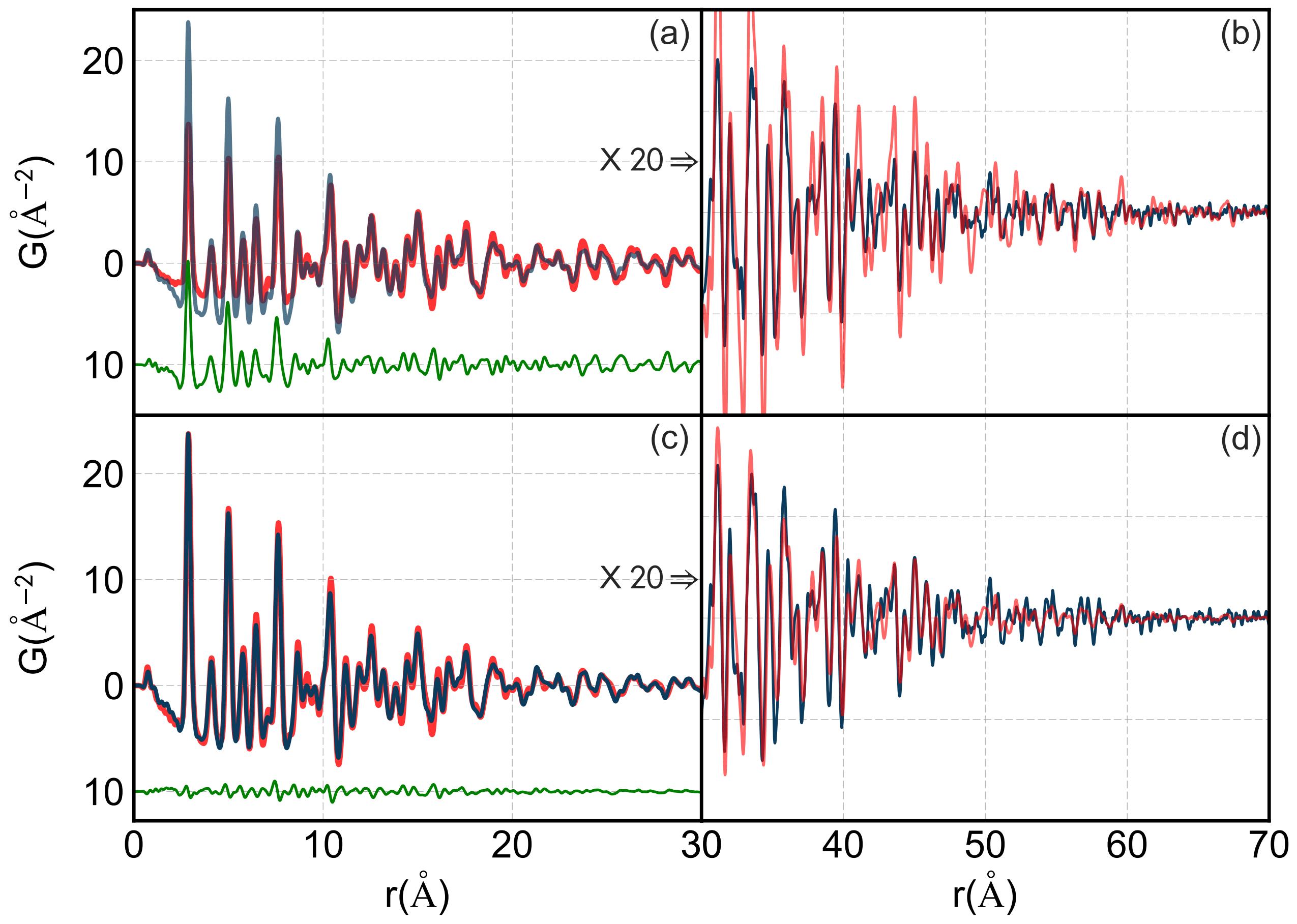


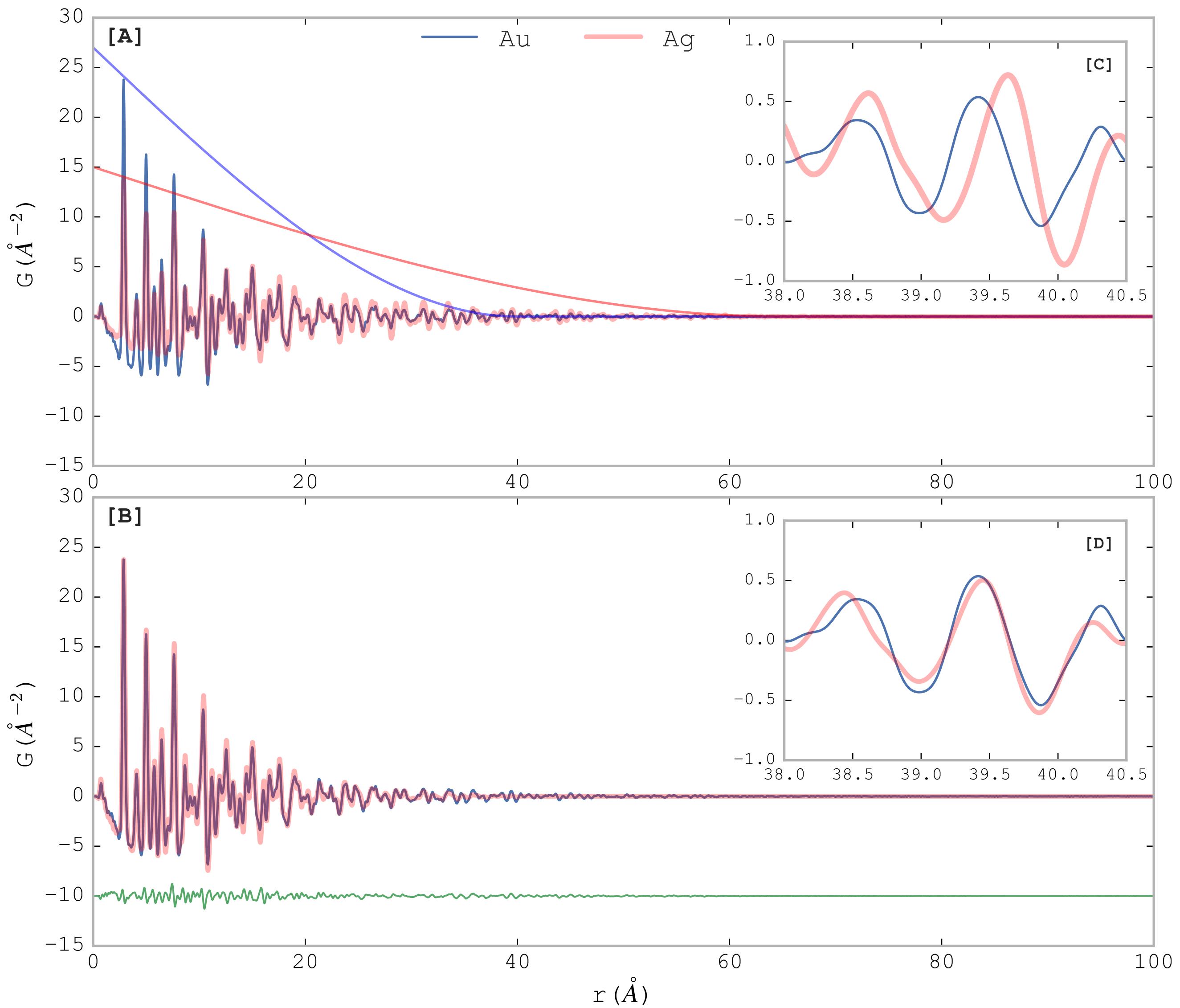
Fig. 5 Representative X-ray powder diffractograms of  $Au$ ,  $Ag : Au\ 50:50$ , and  $Ag$  nanoparticles. At the bottom, the peaks of elemental silver are indicated. Note the traces of  $AgCl$  from the synthesis which were found in pure silver nanoparticles.

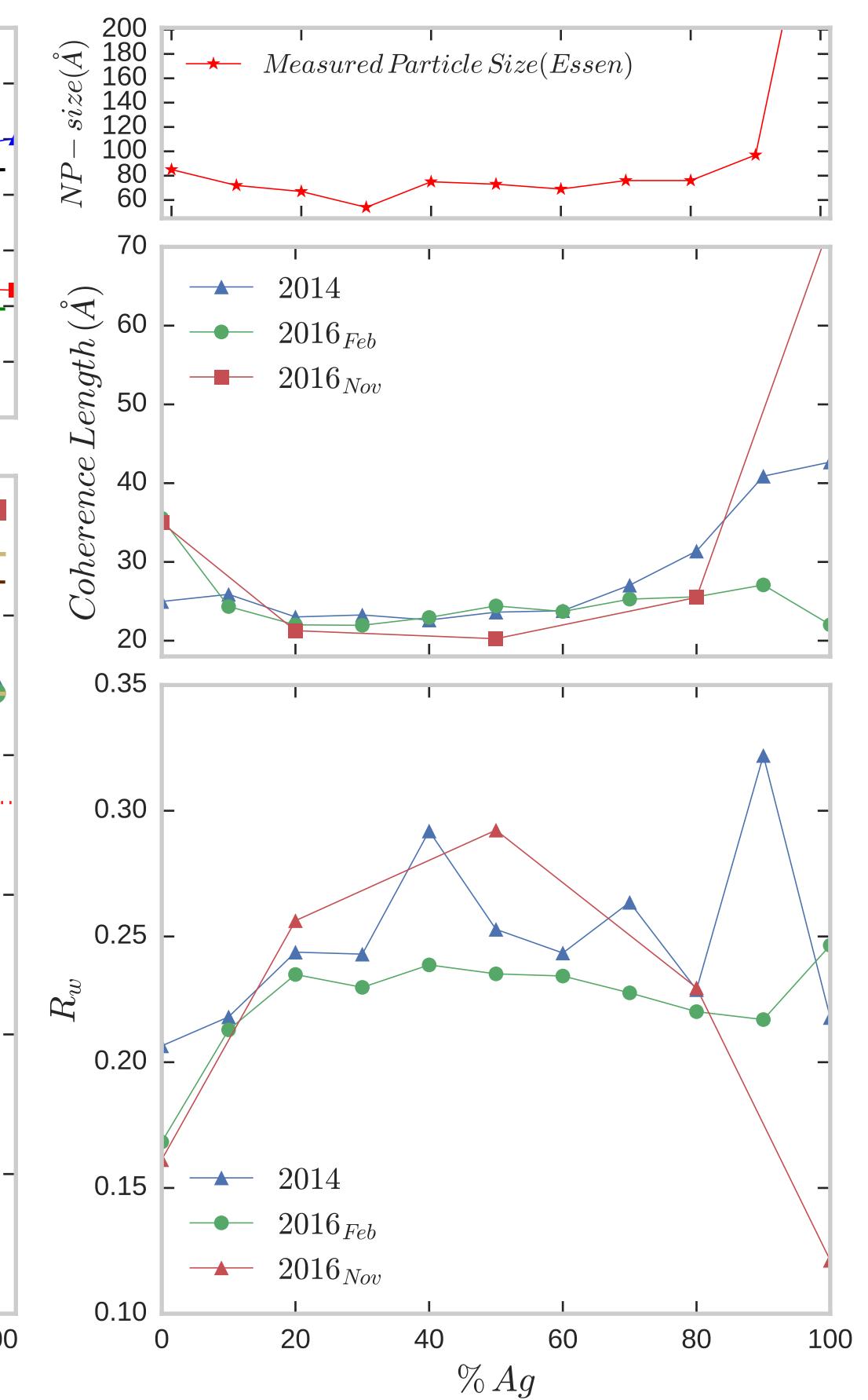
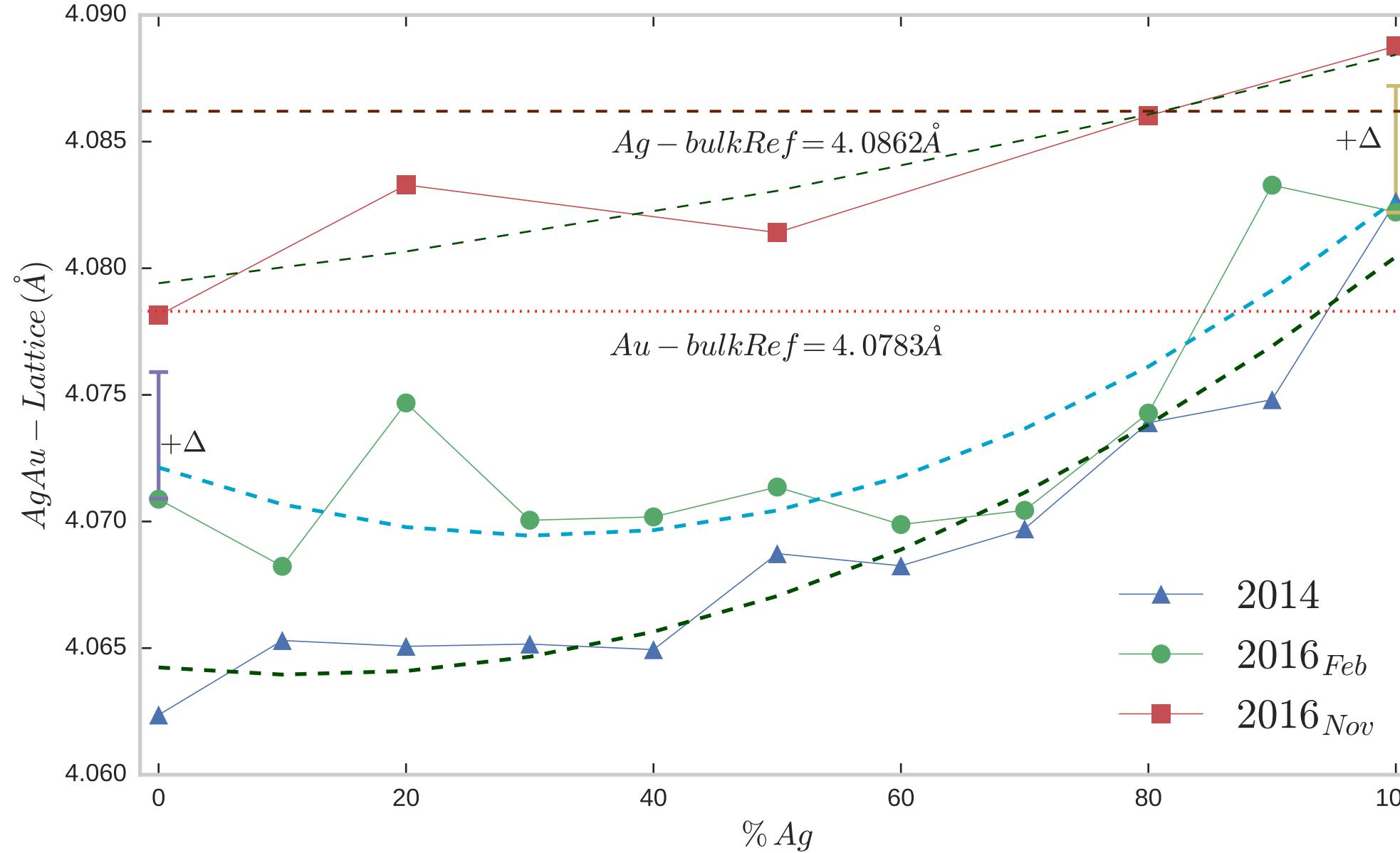
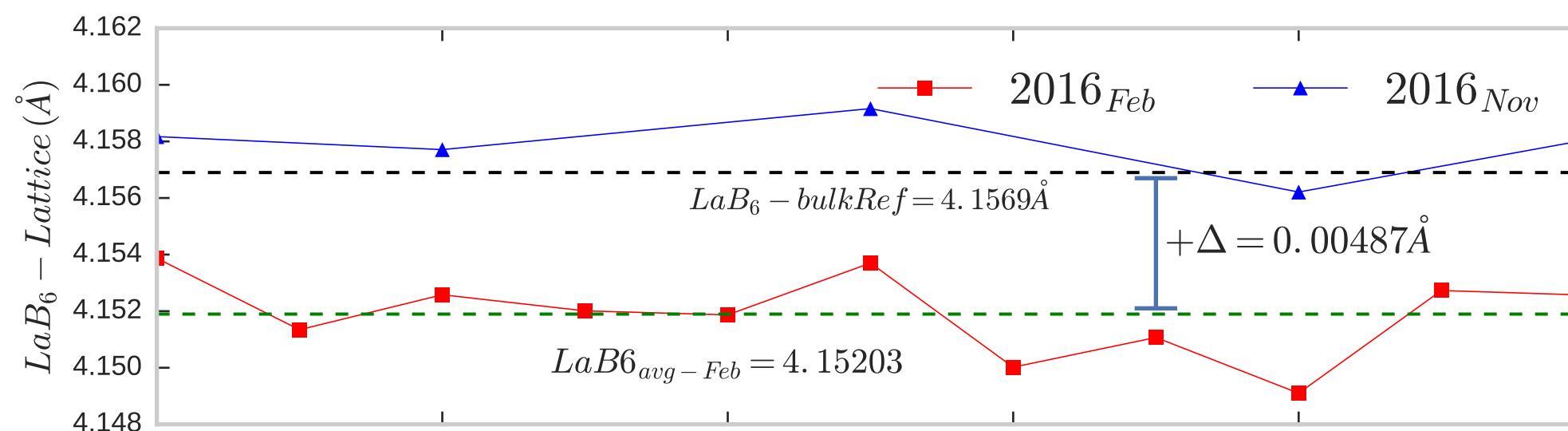


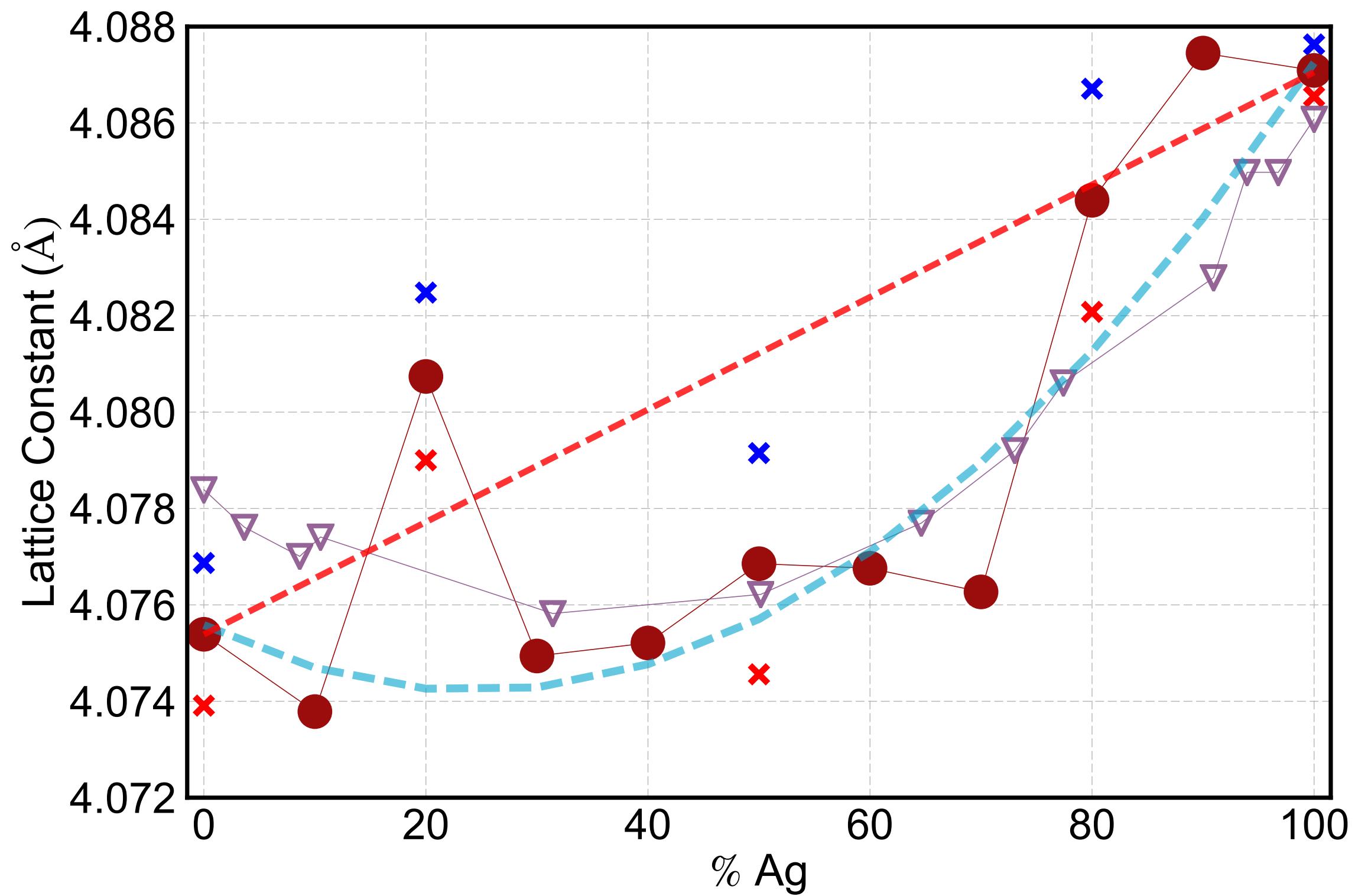


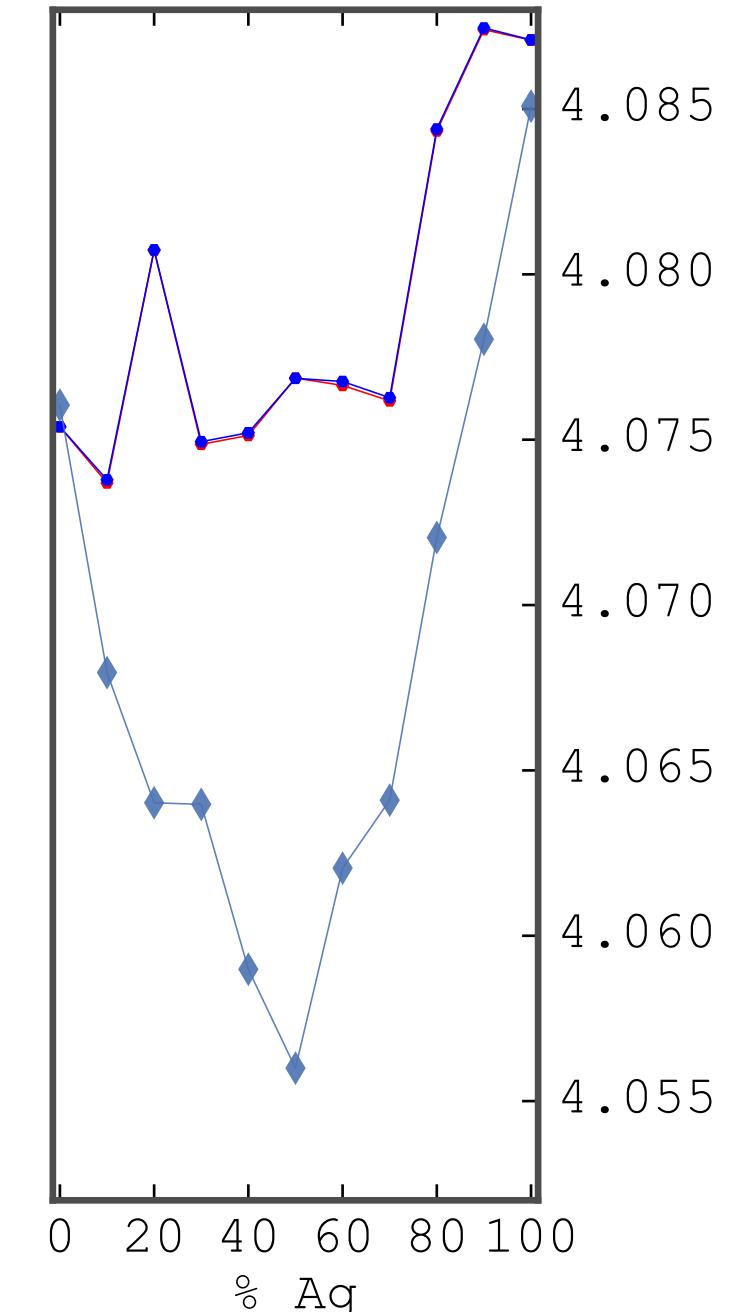
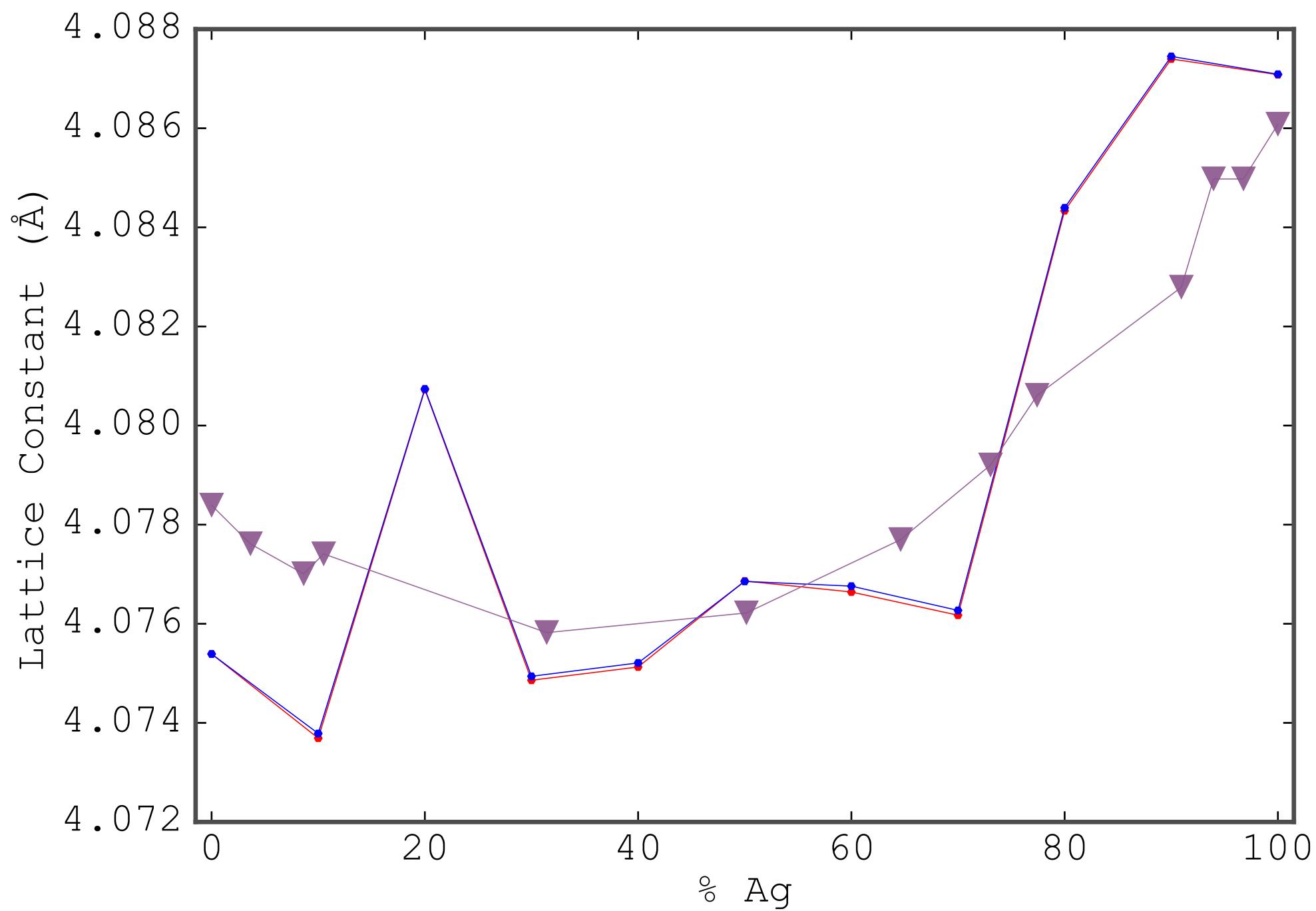


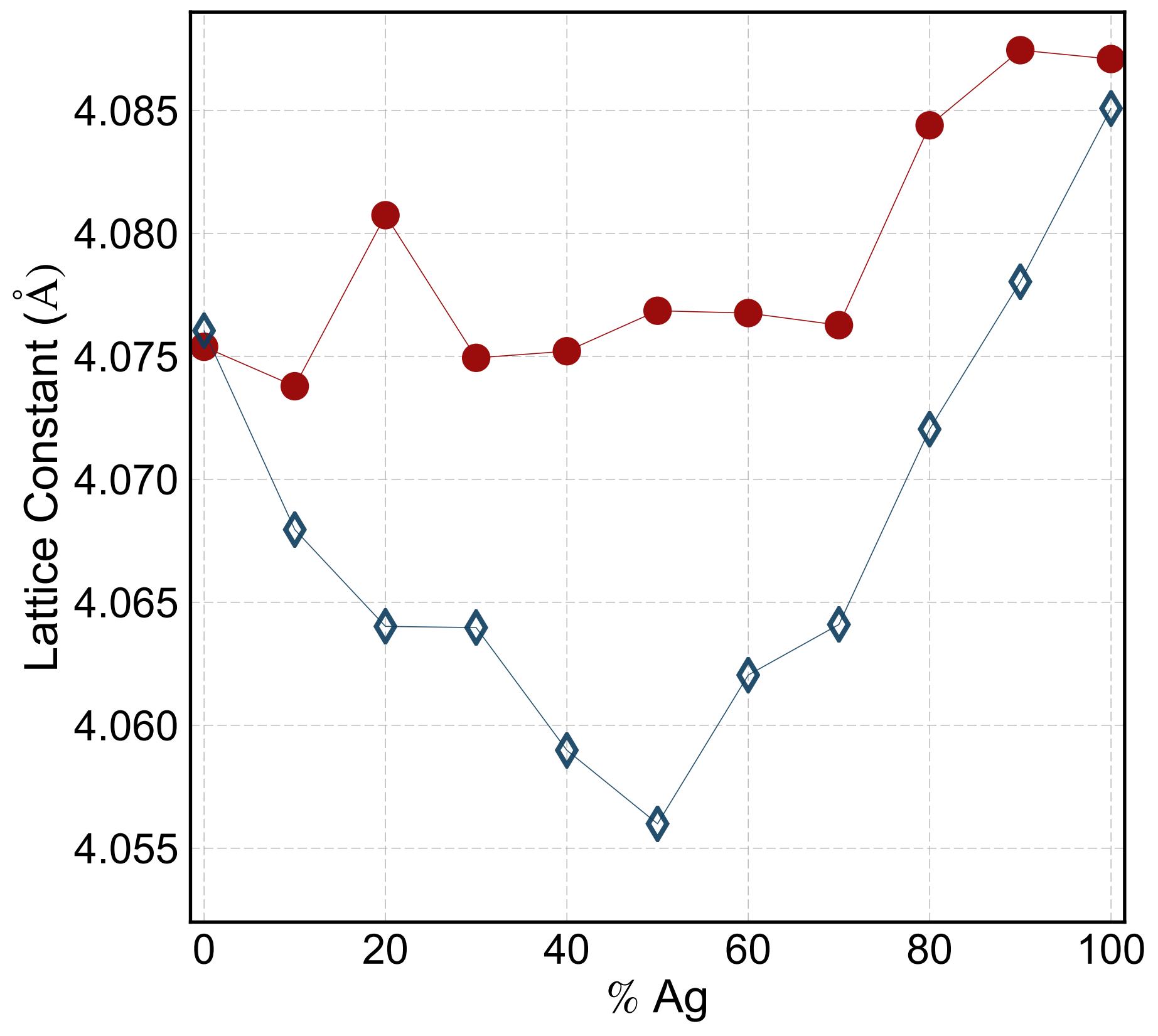


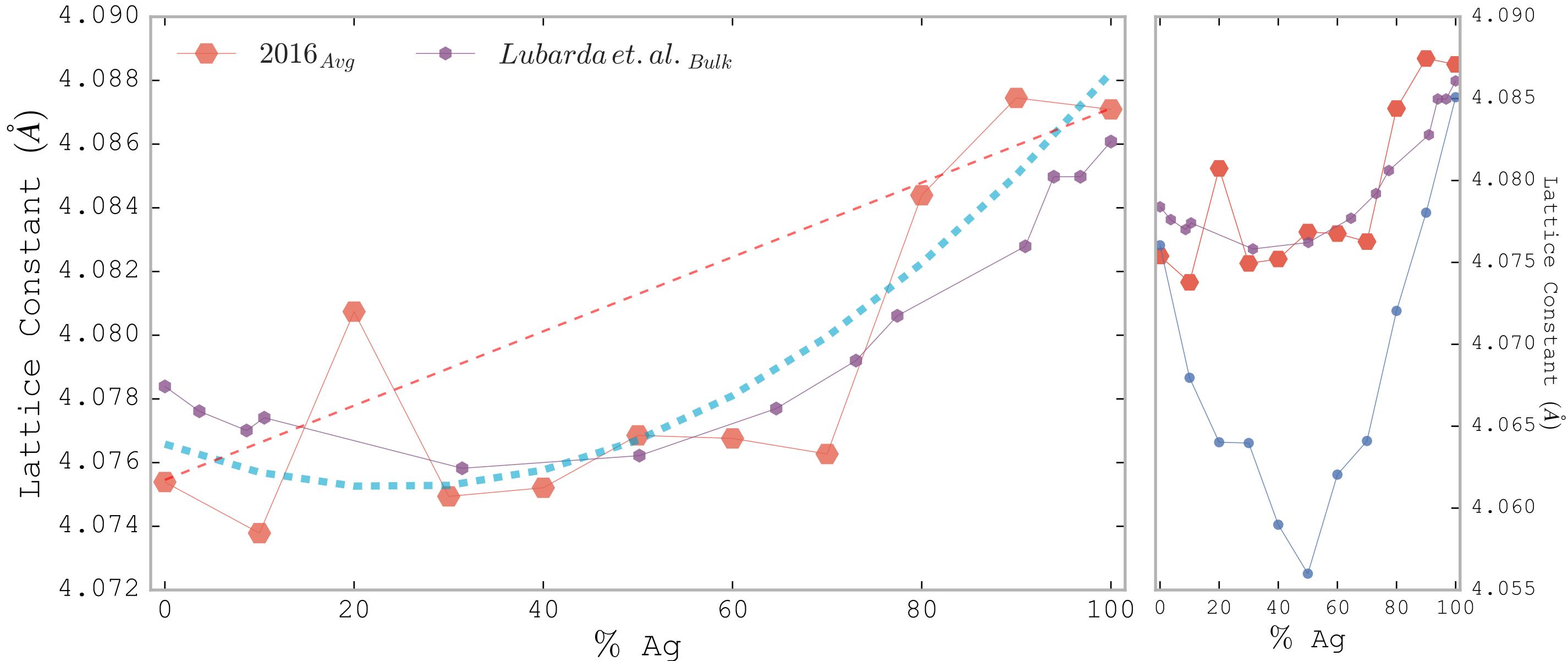


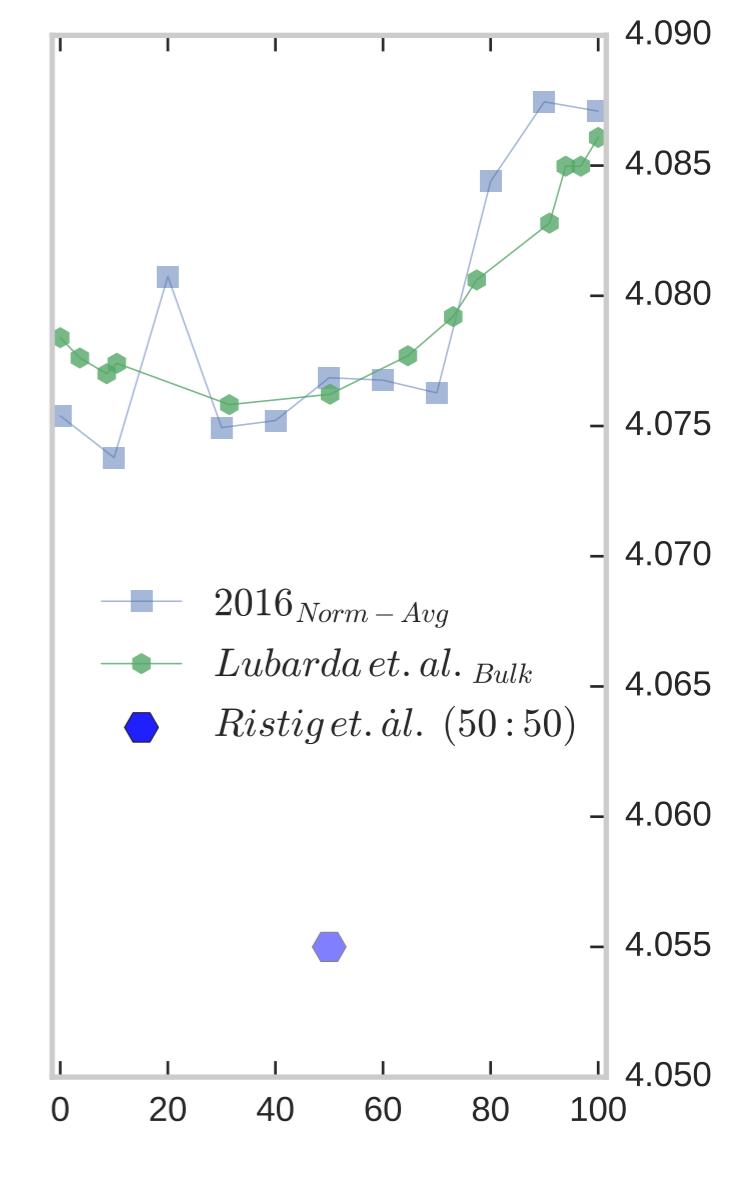
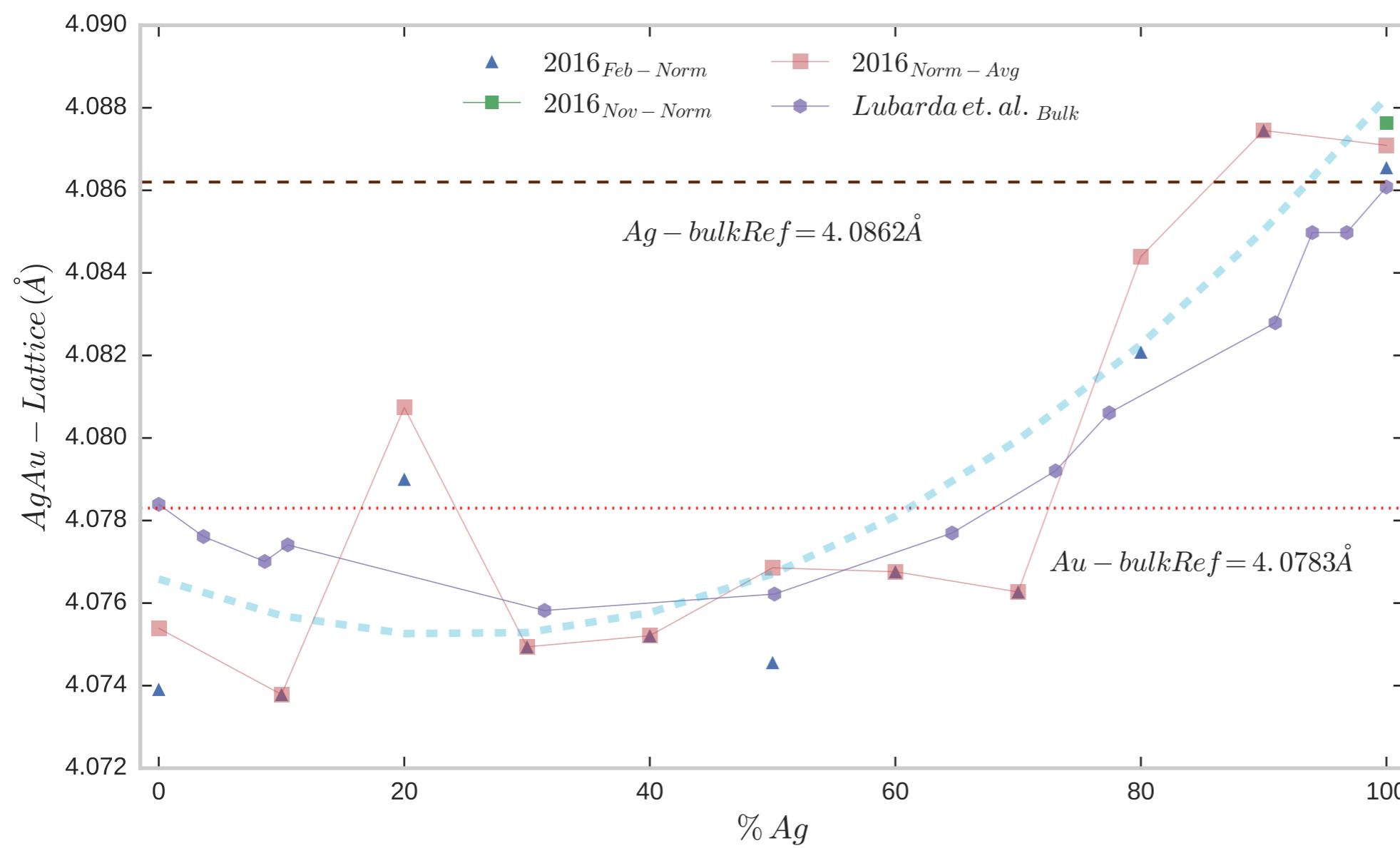


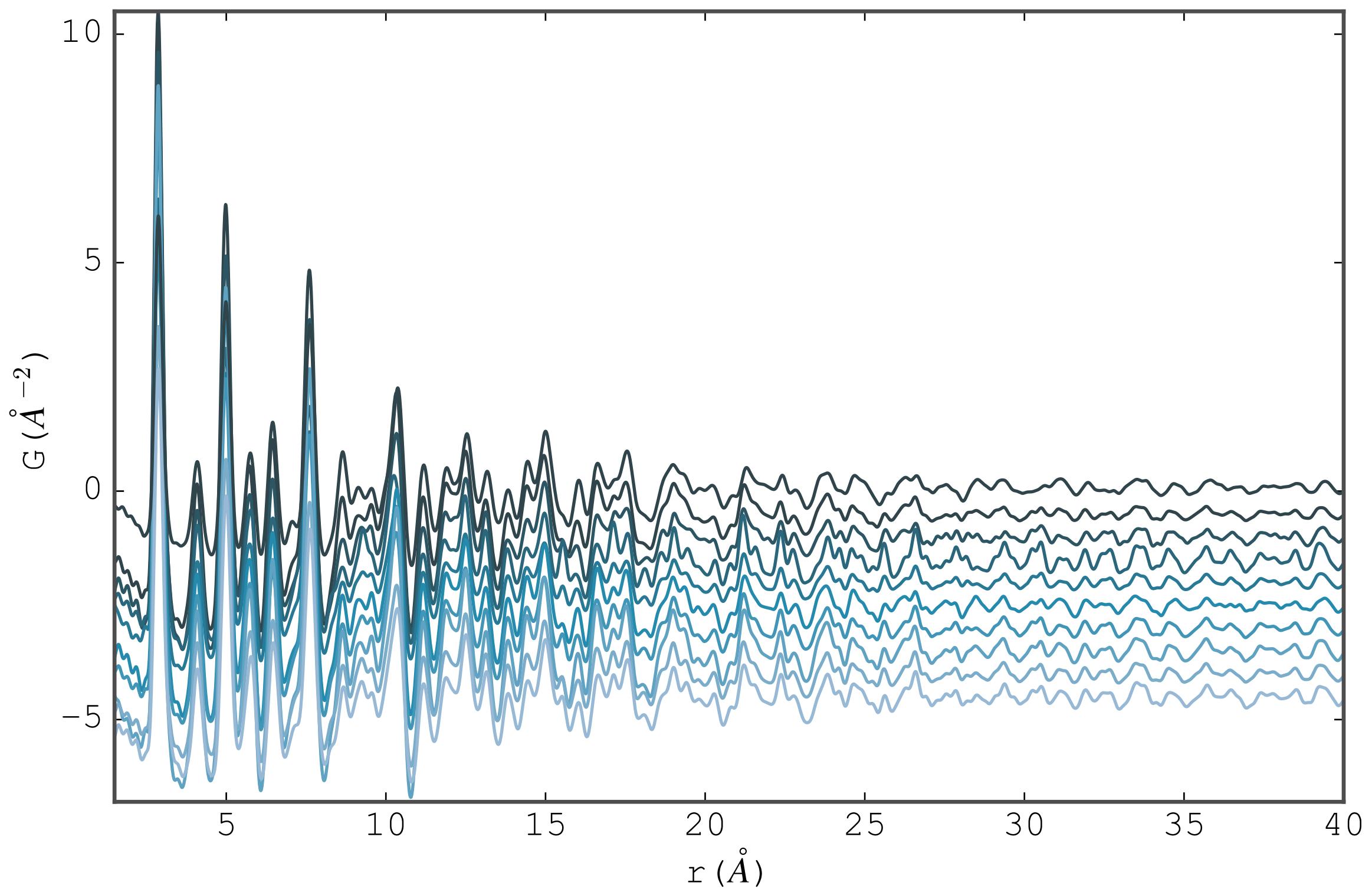


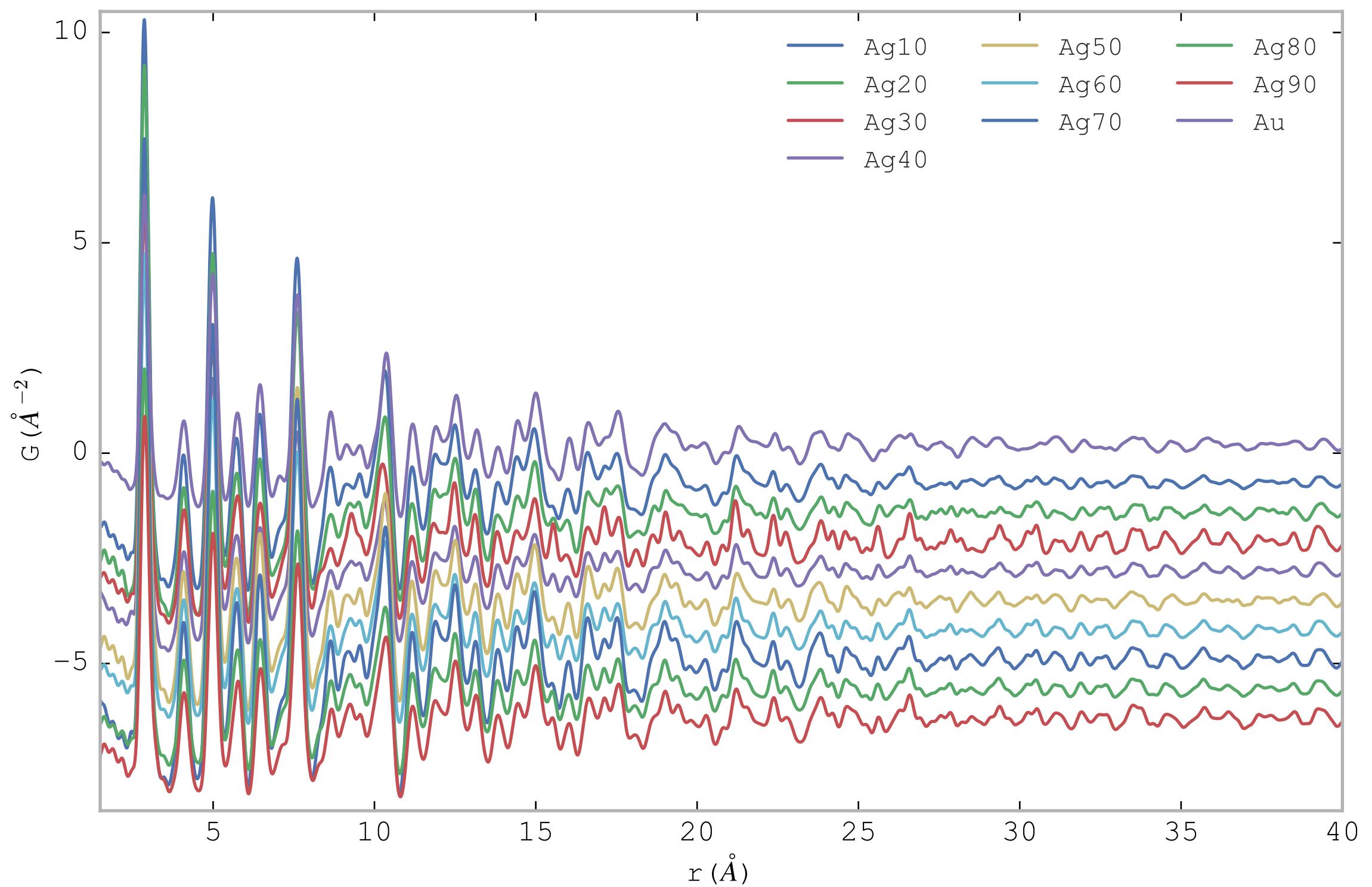


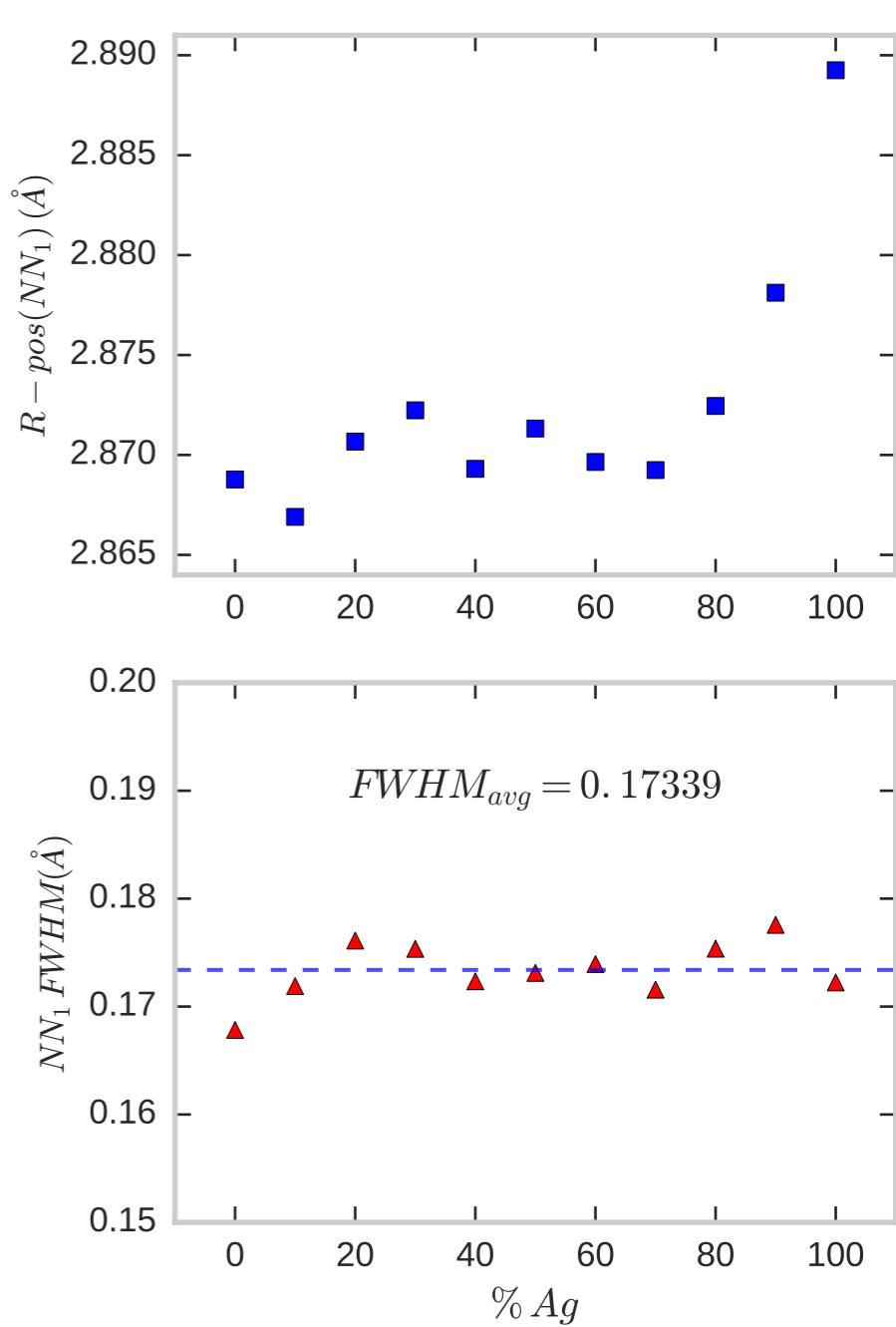
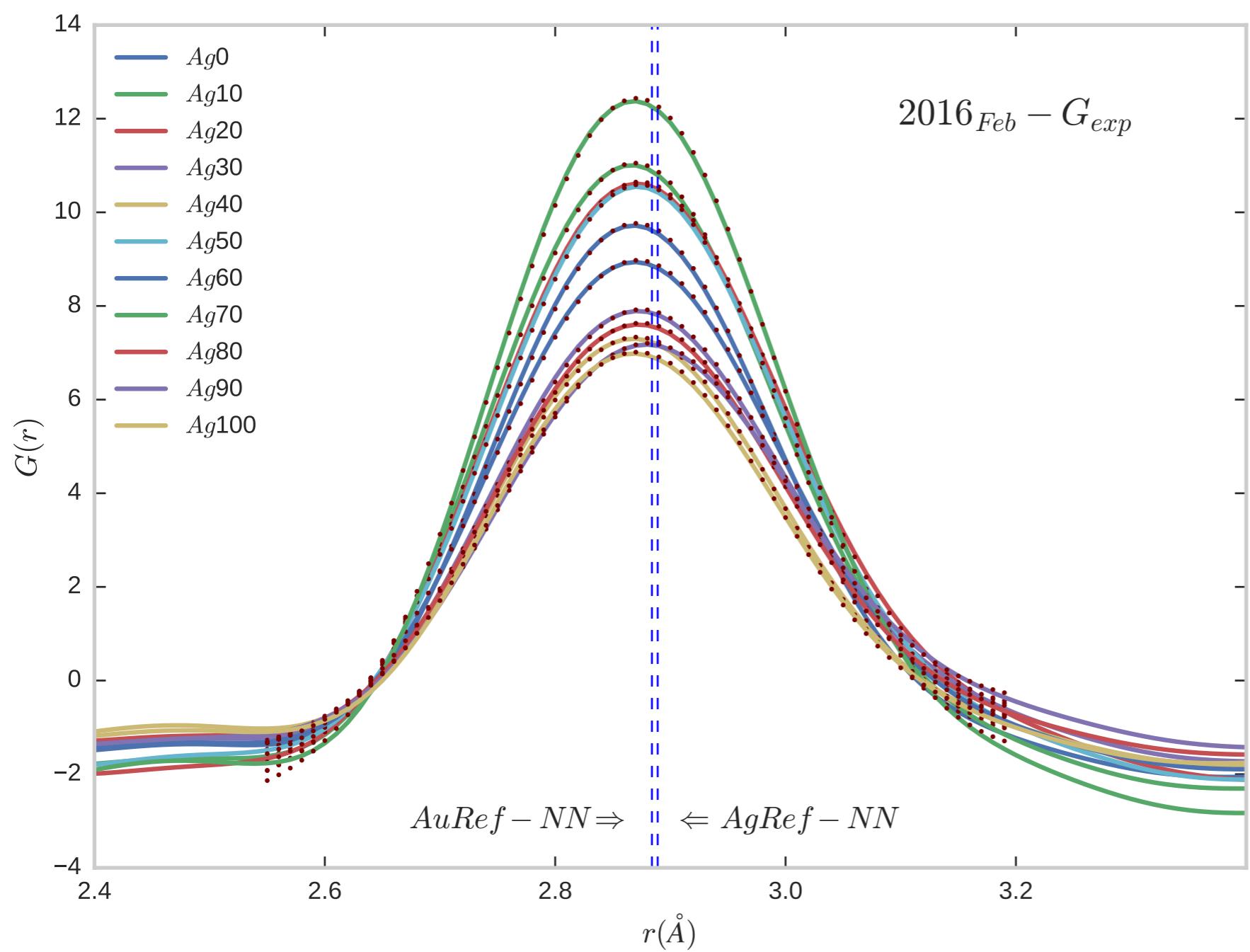


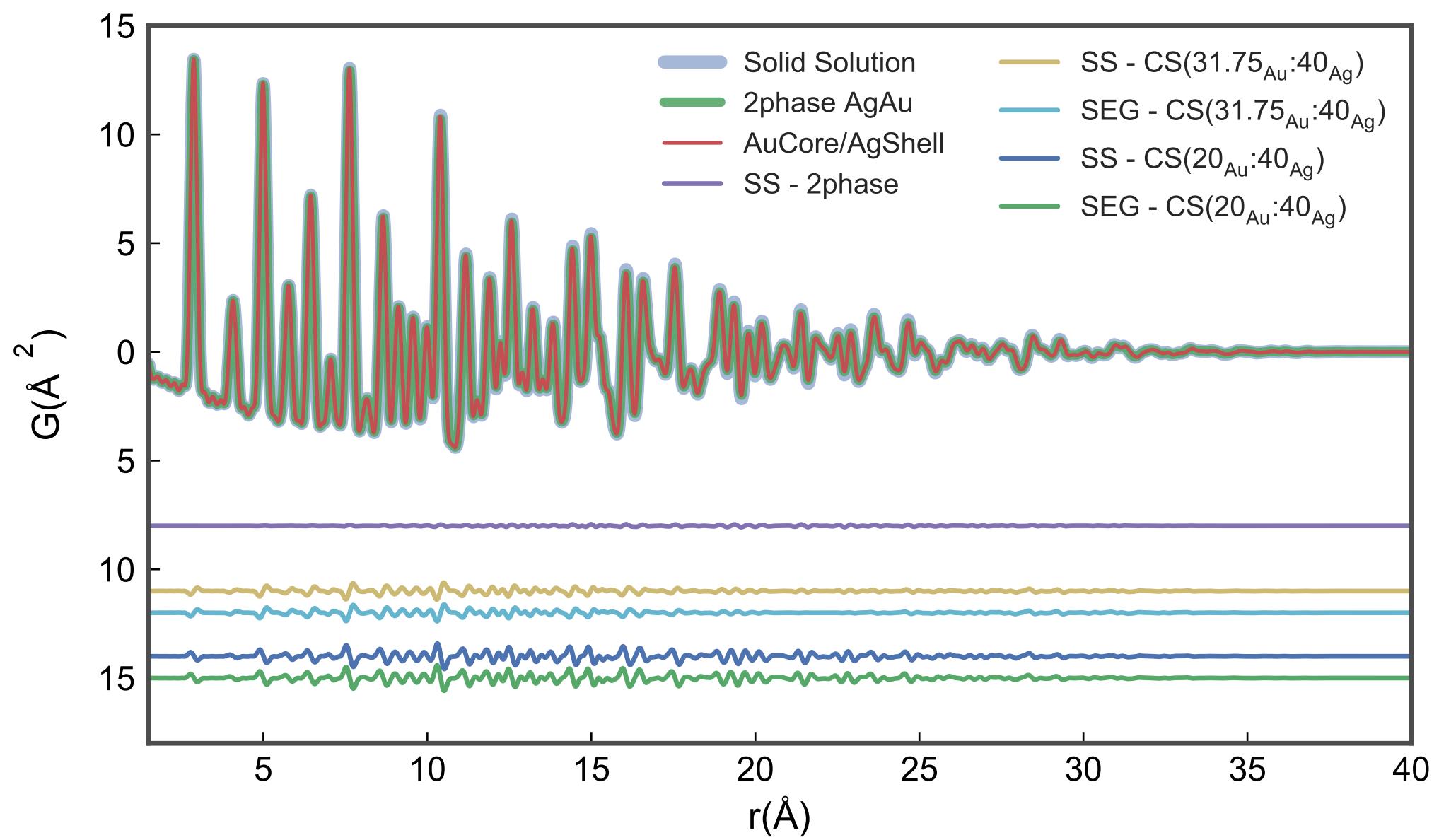


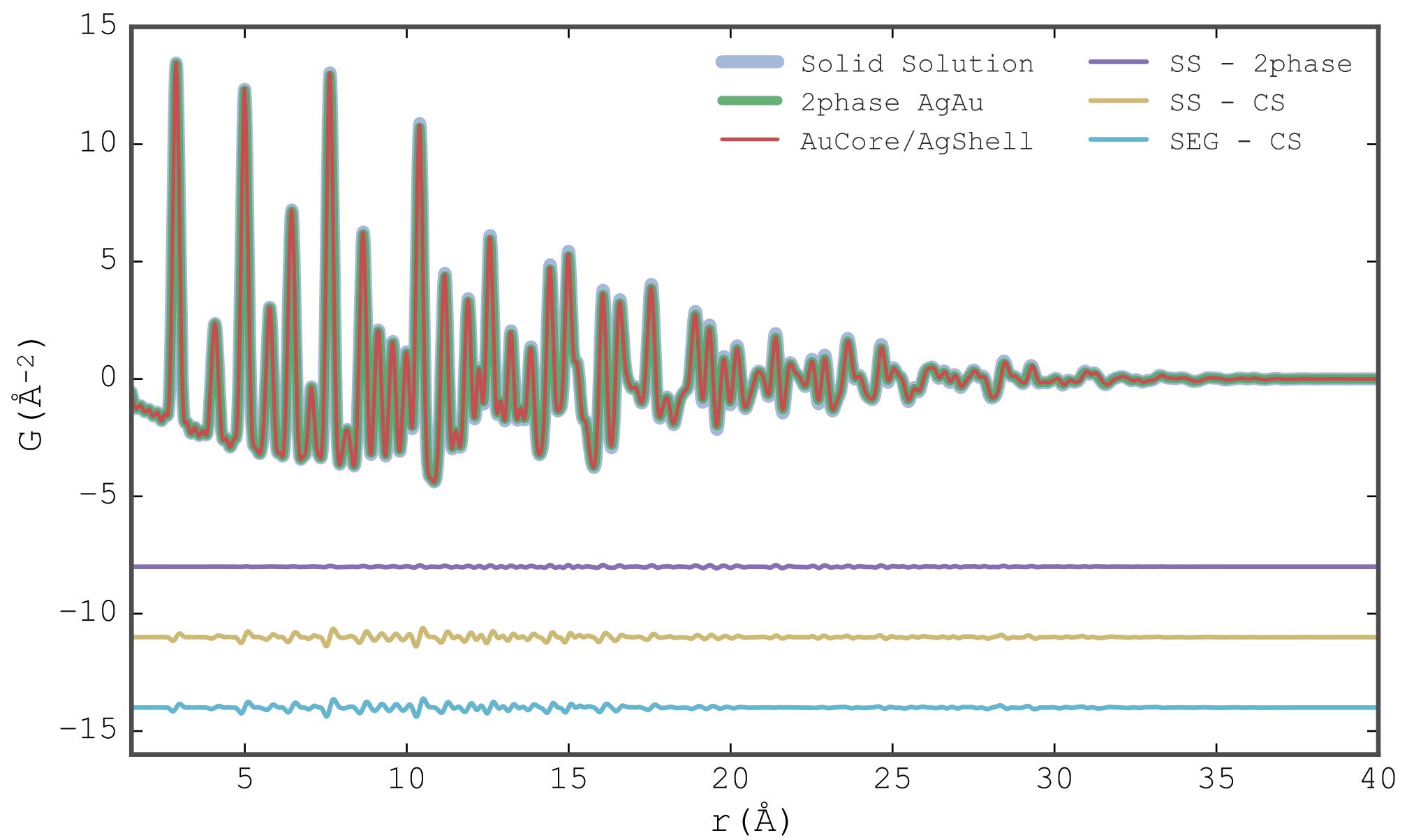


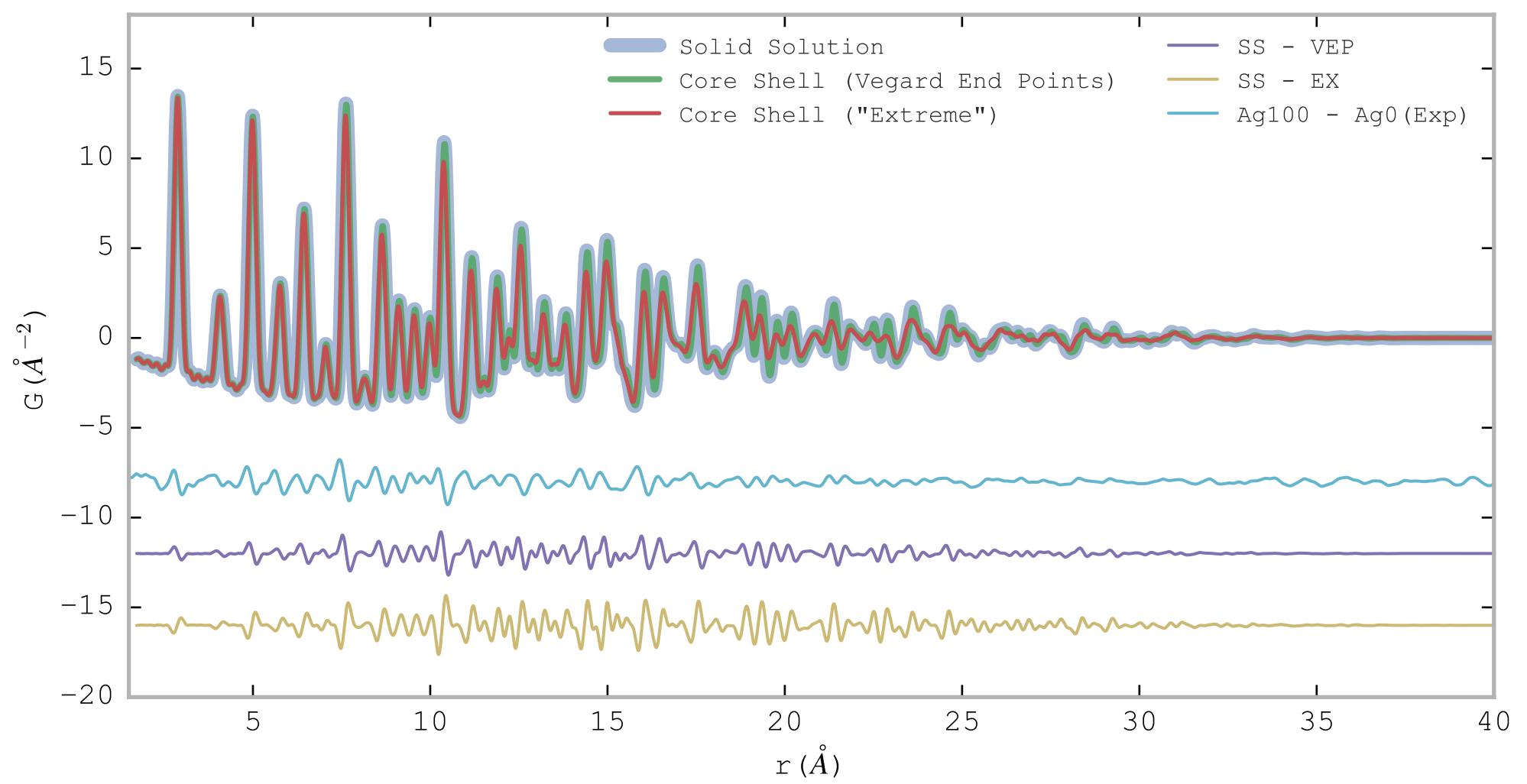


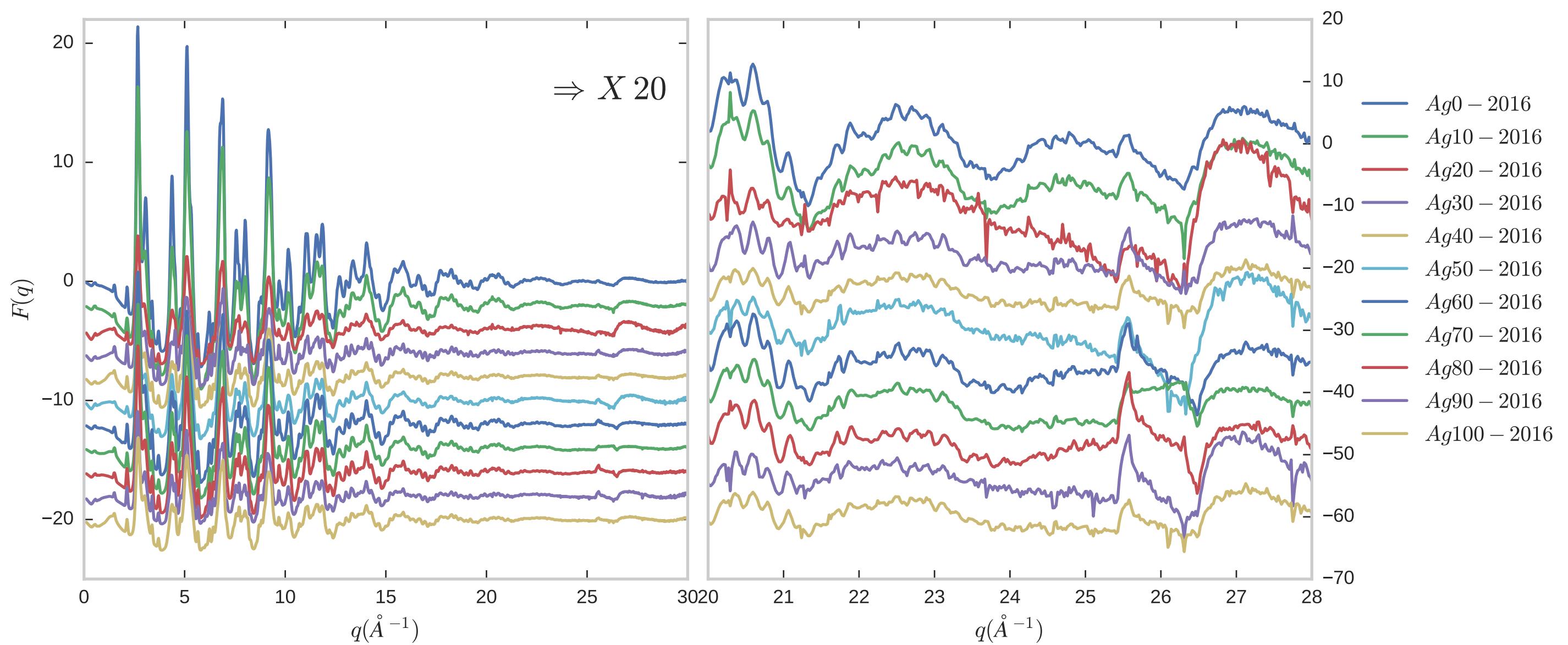


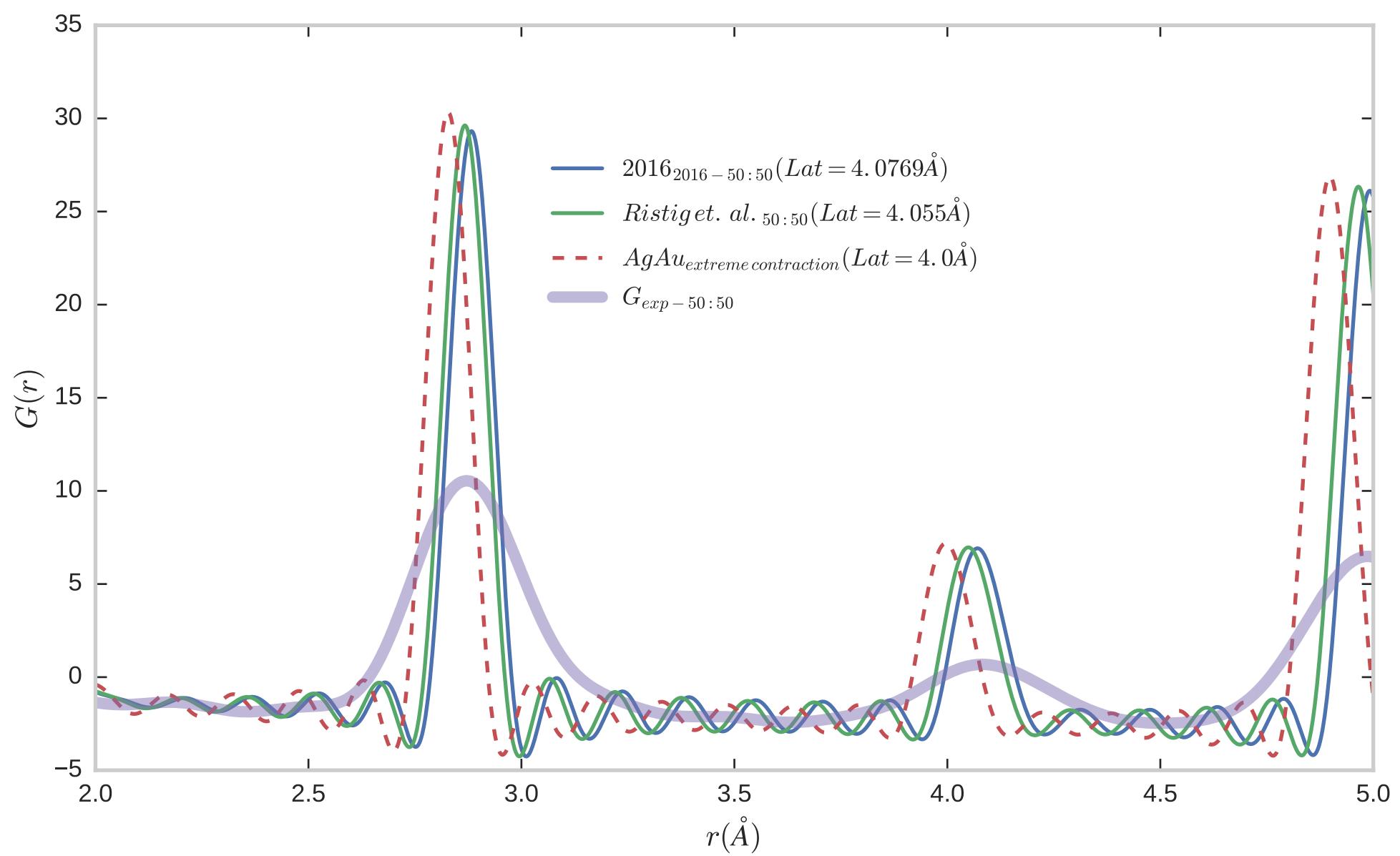


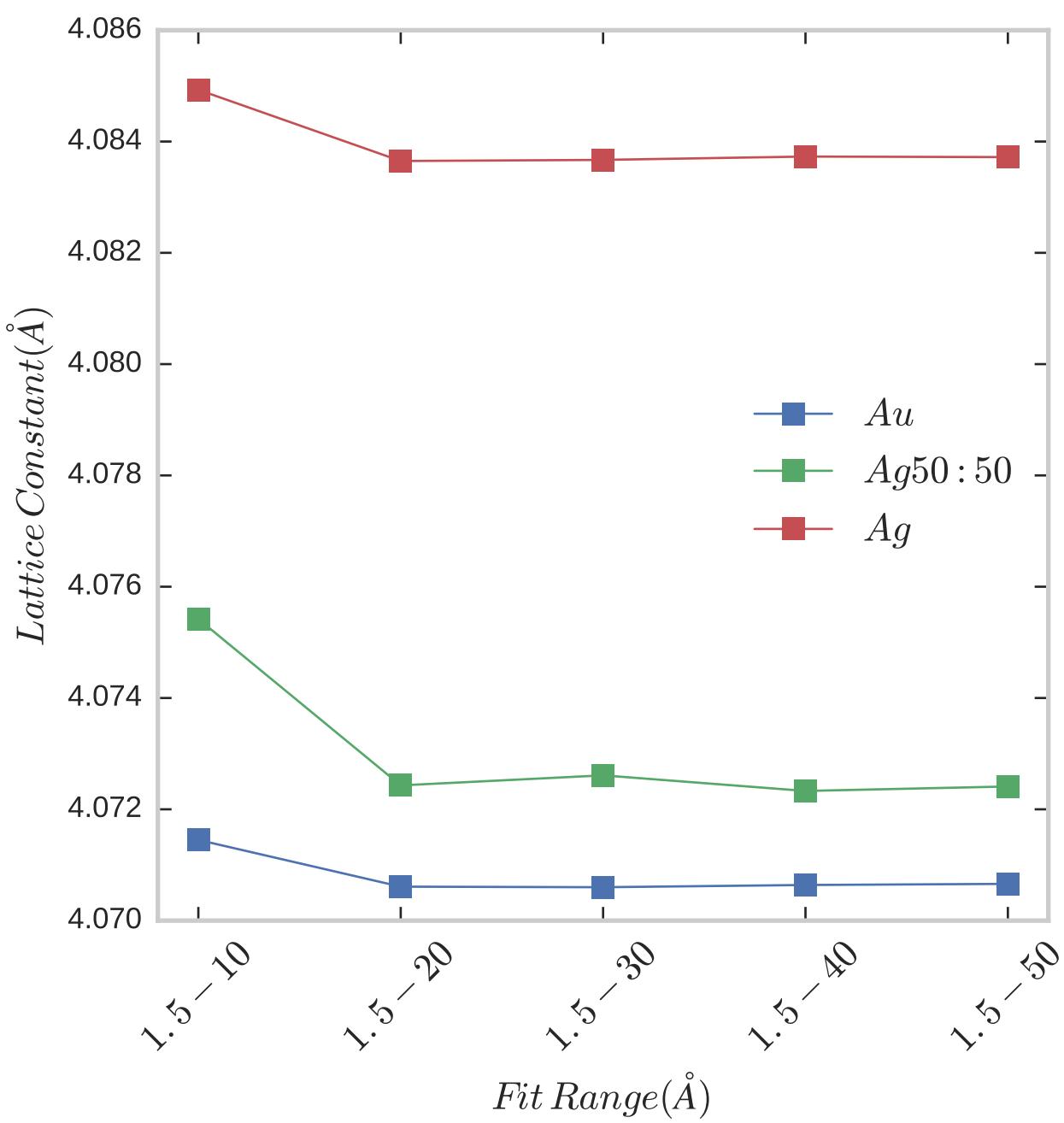


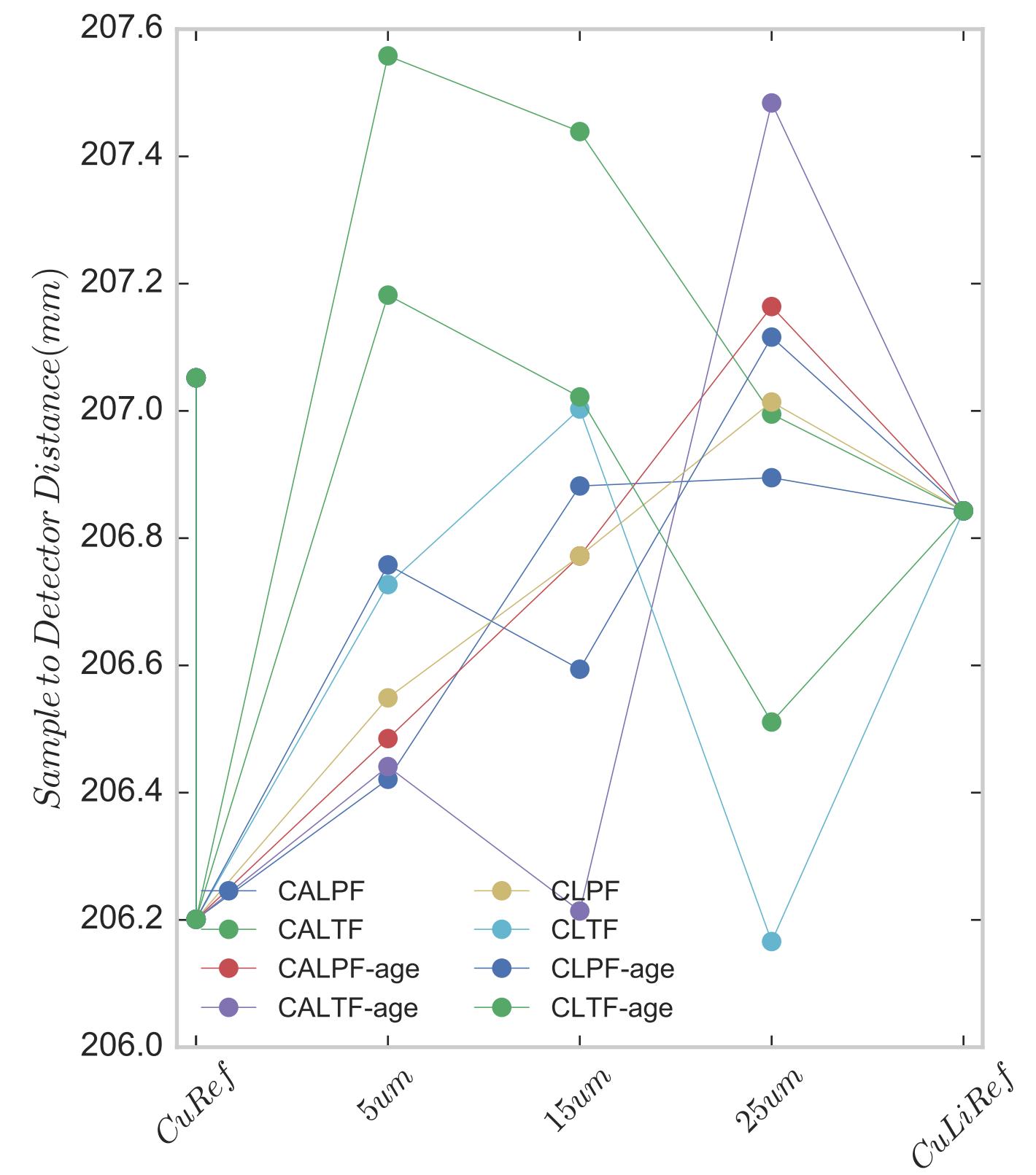
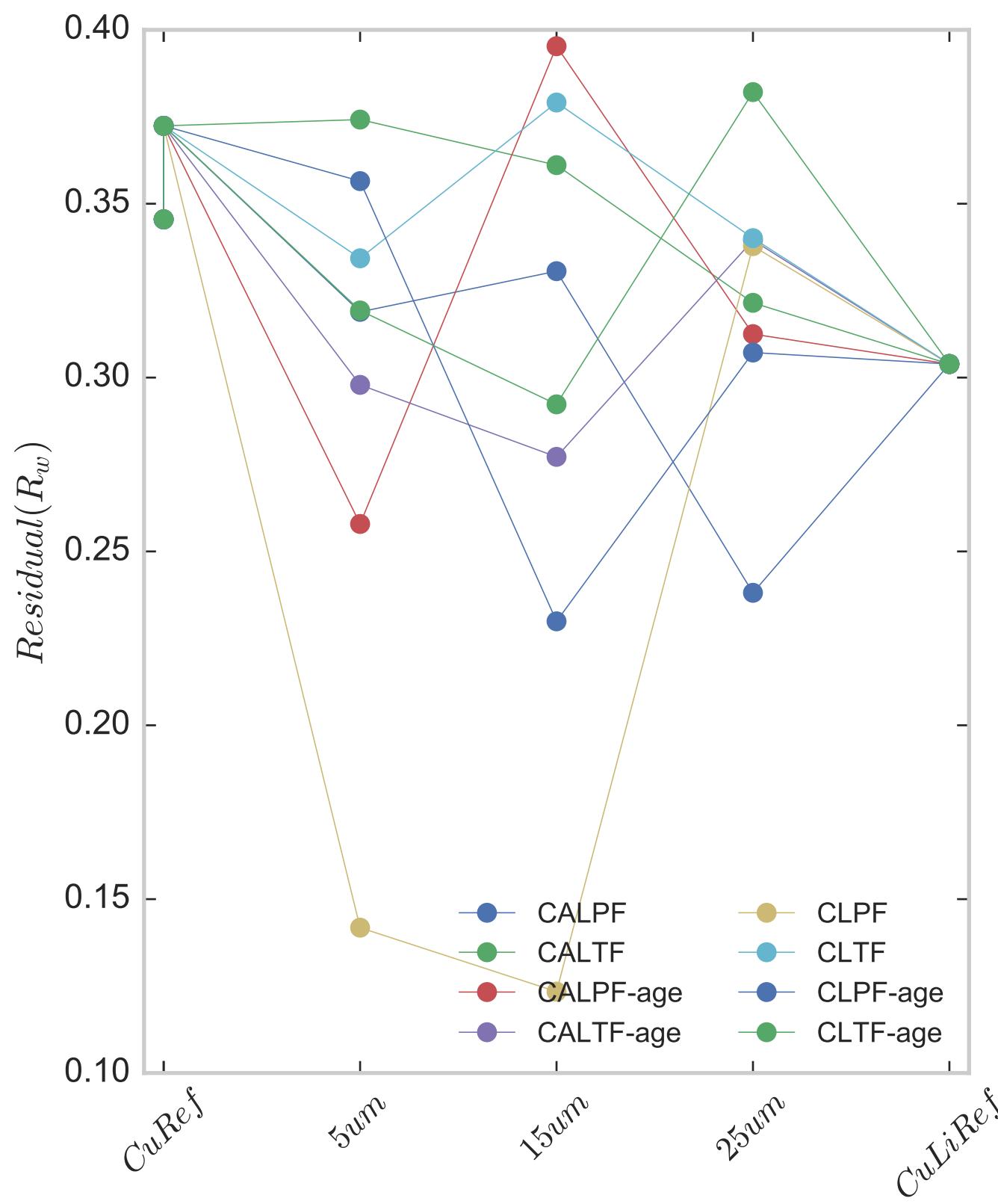


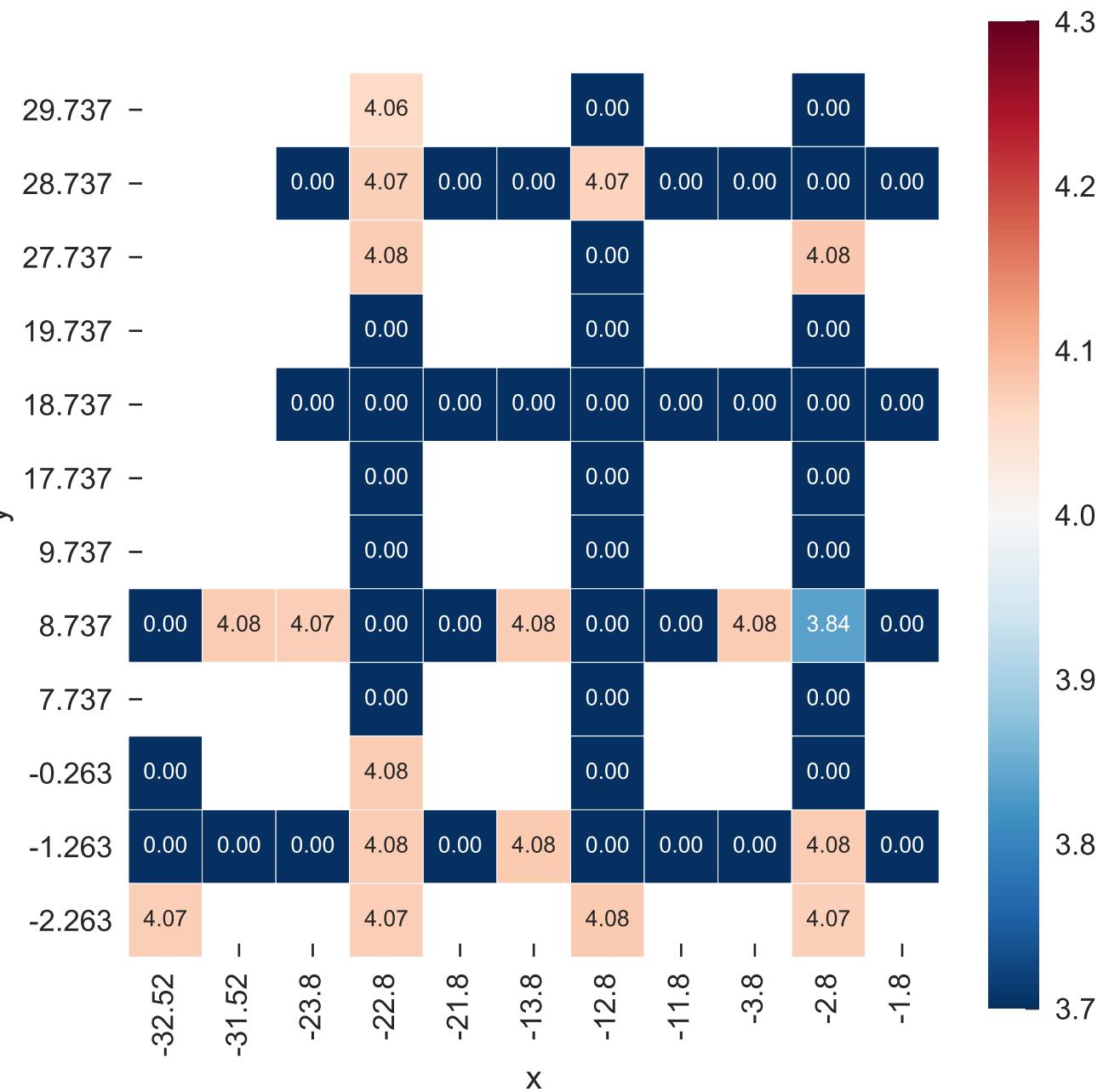


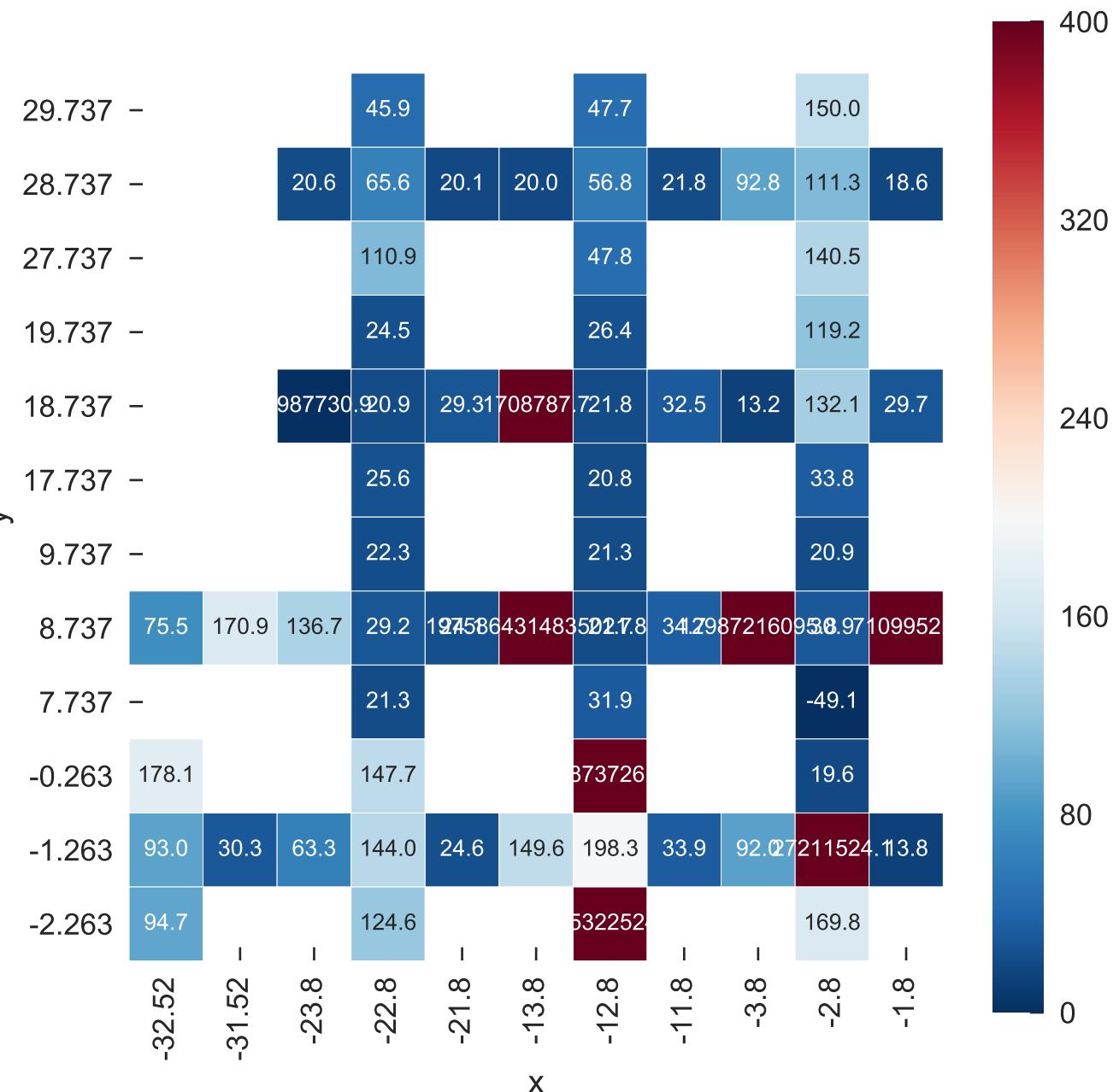


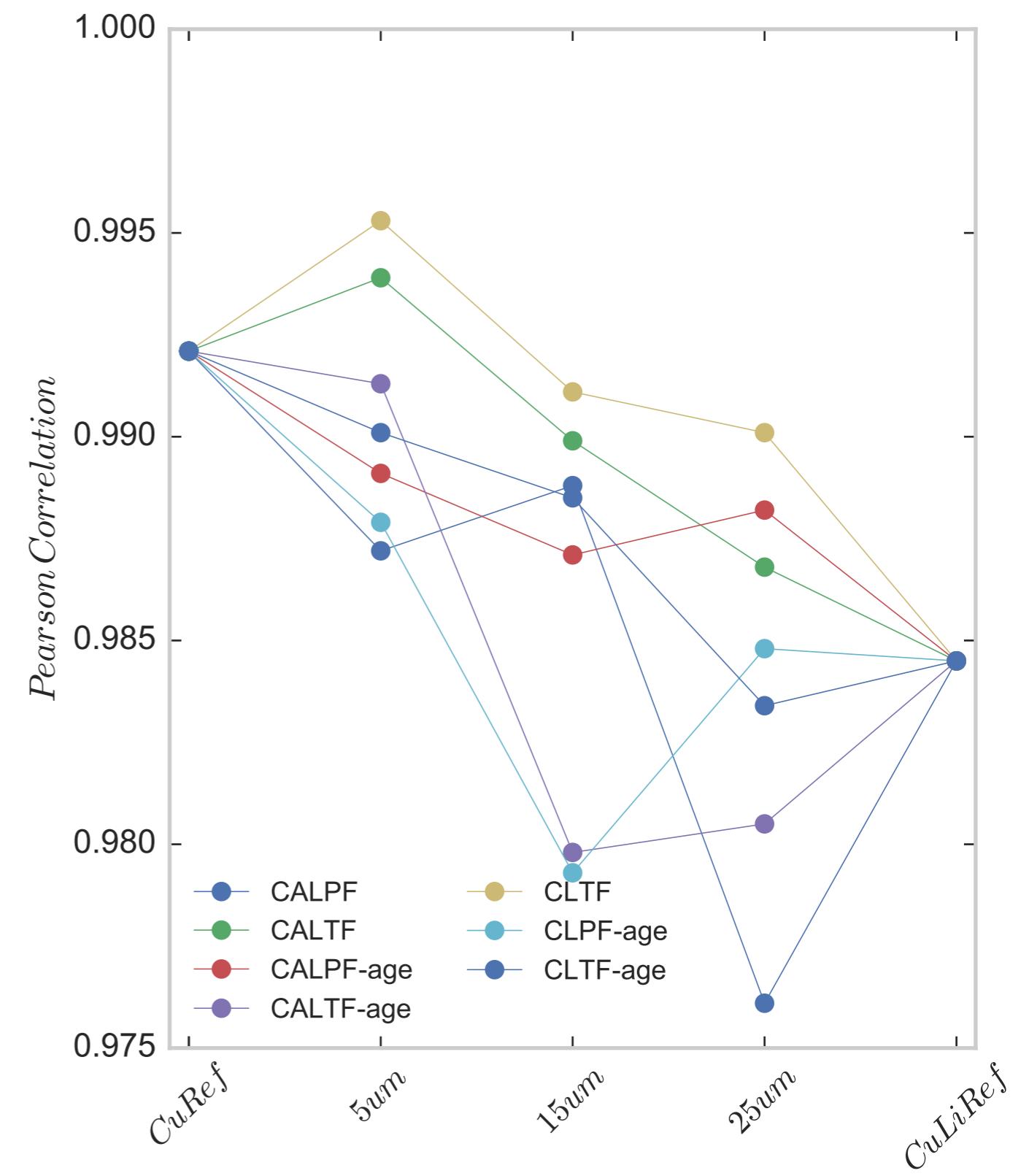
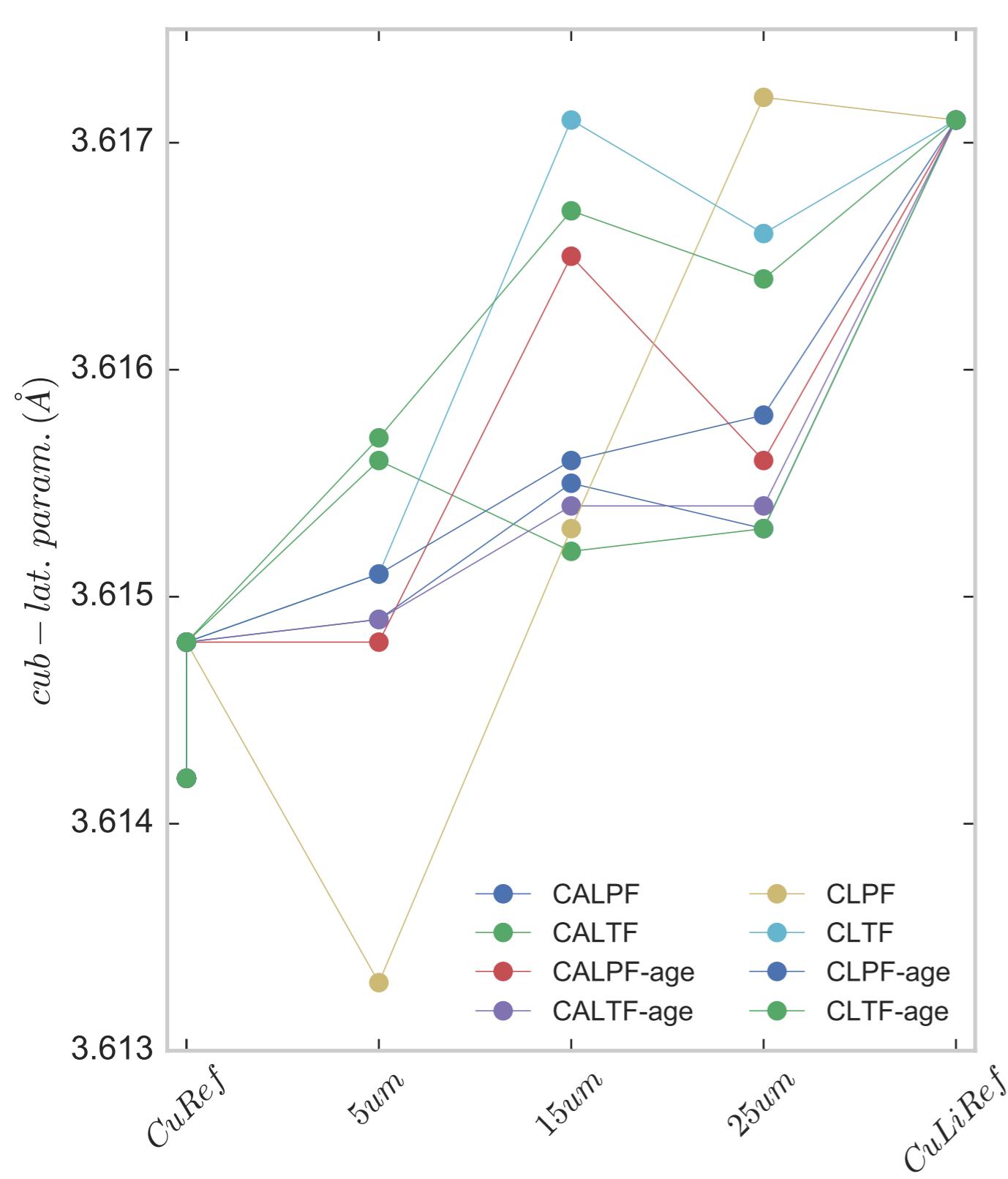




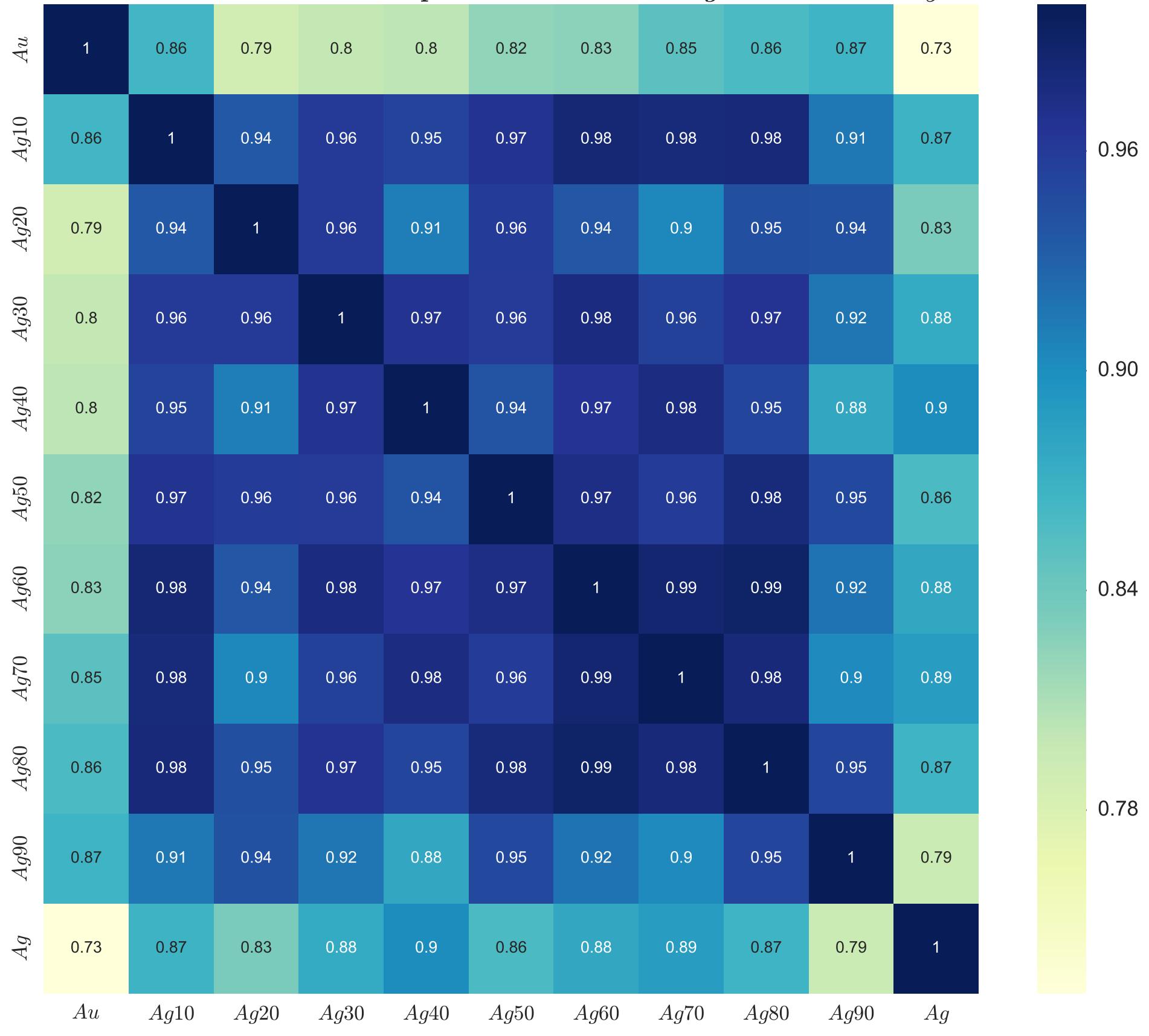


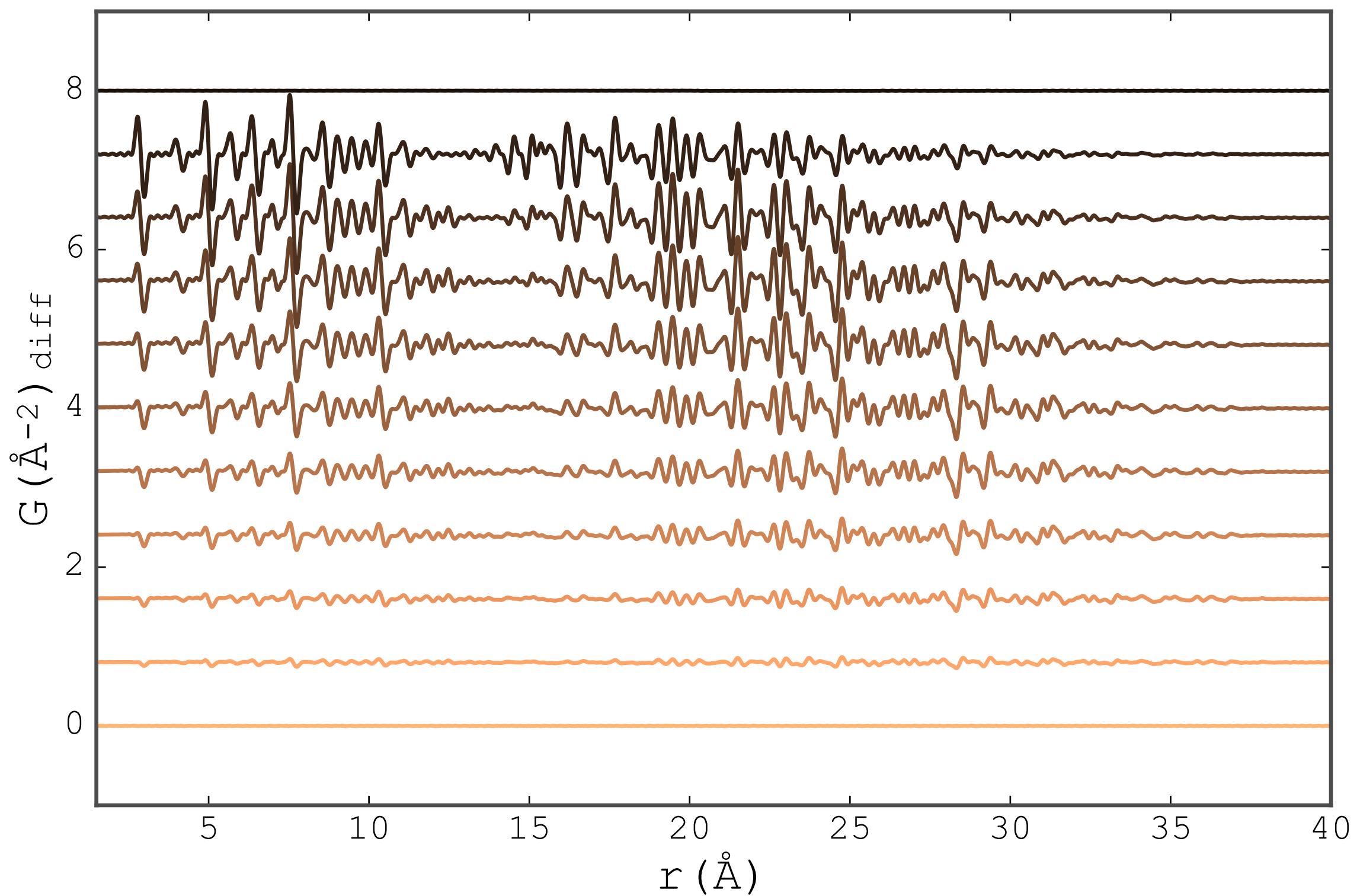


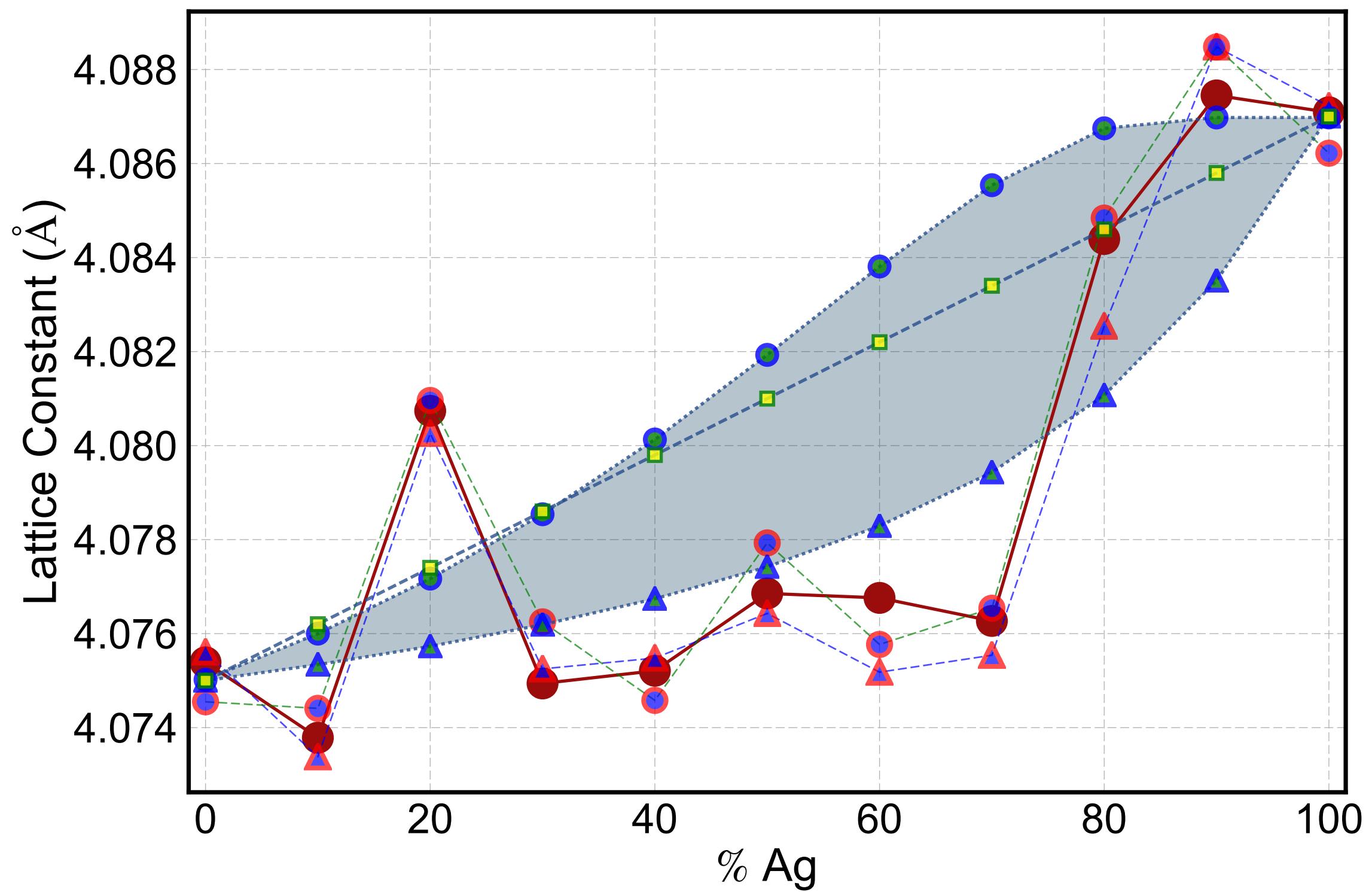


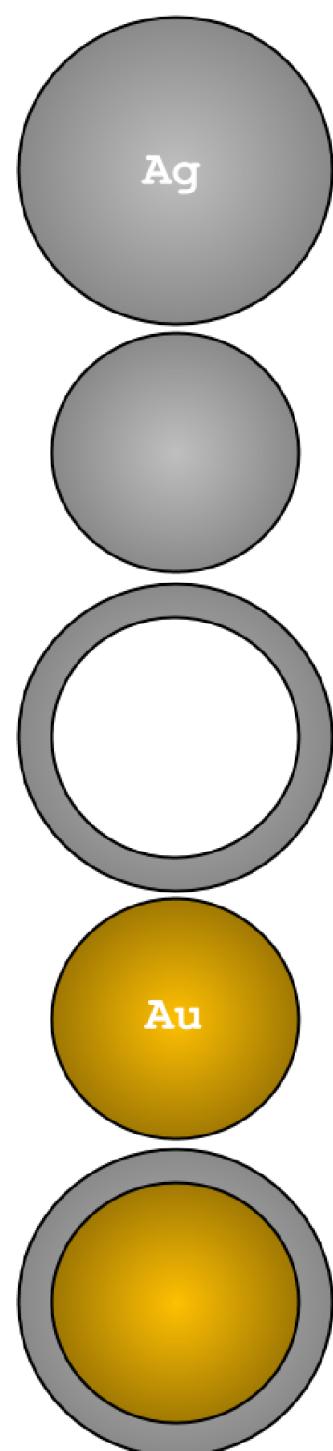
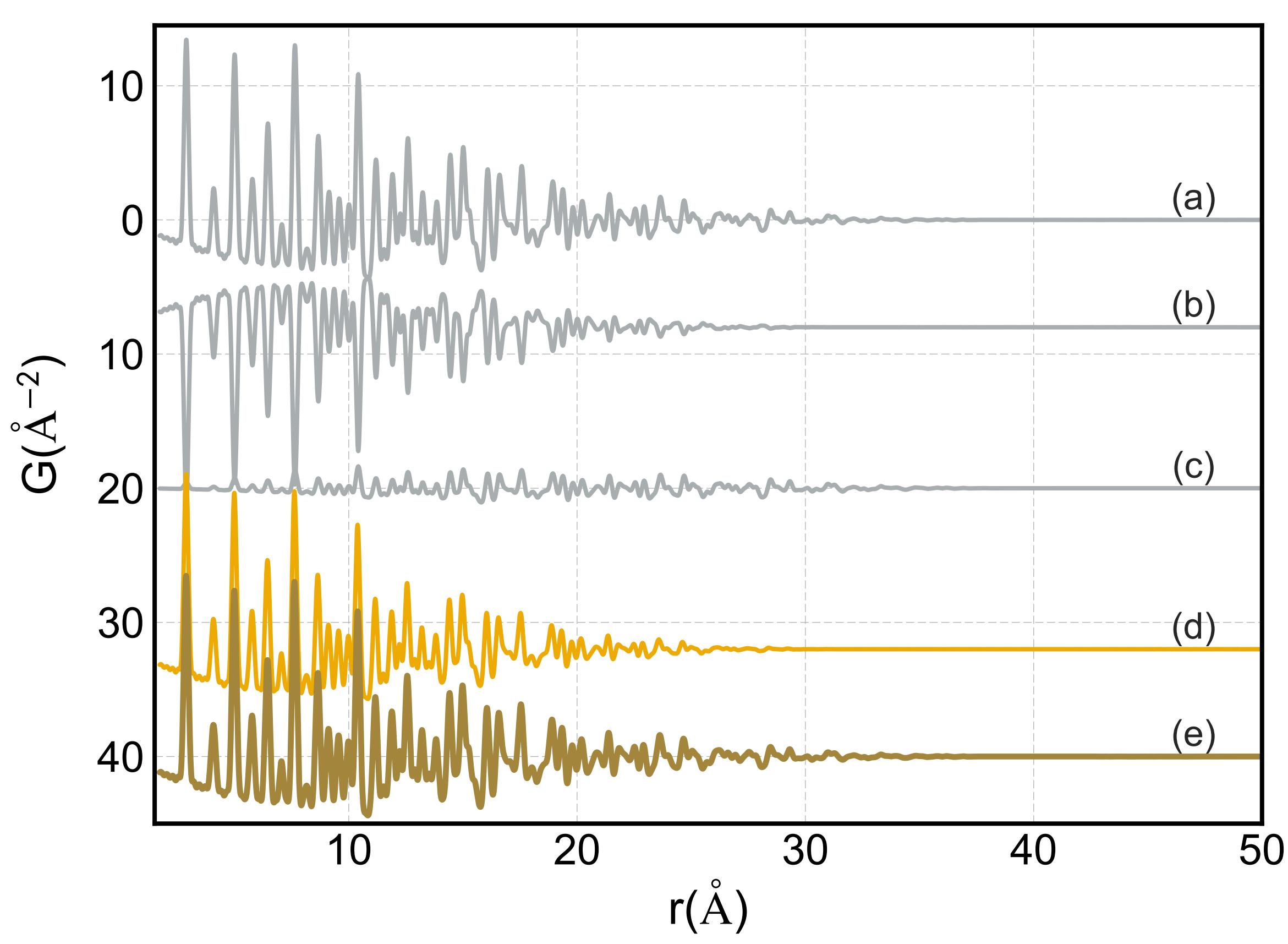


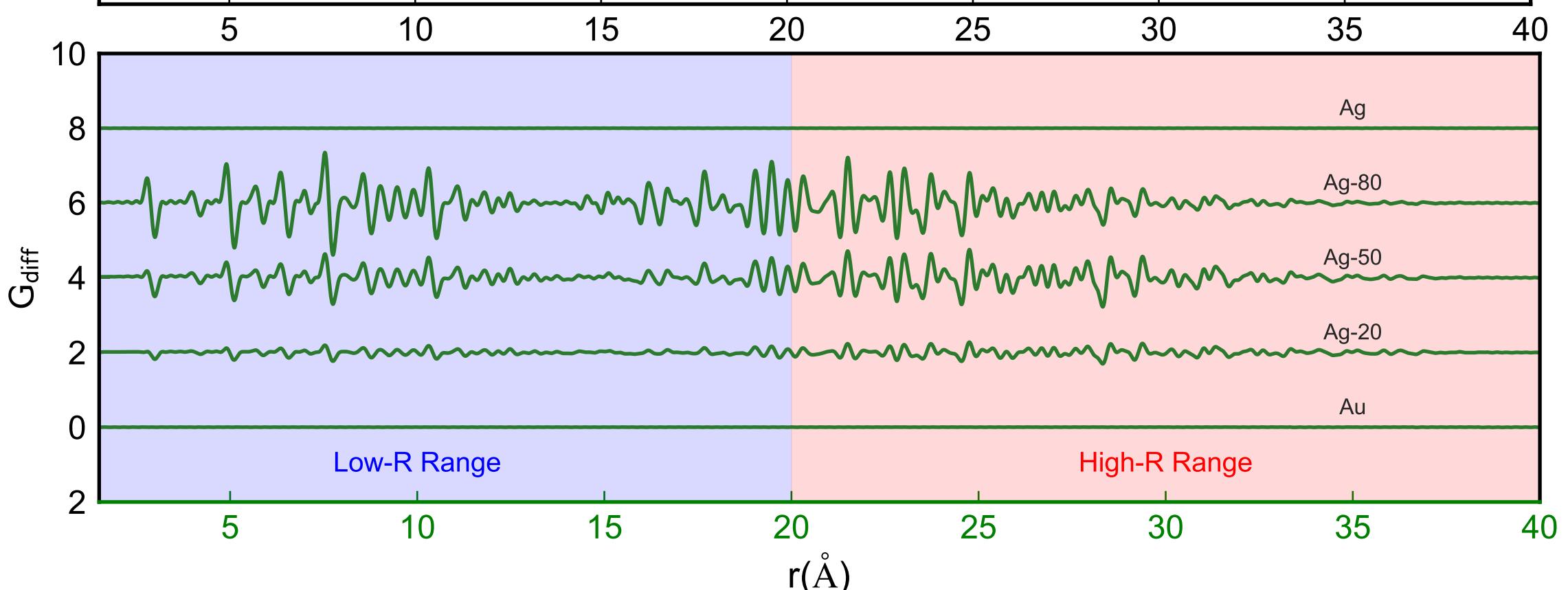
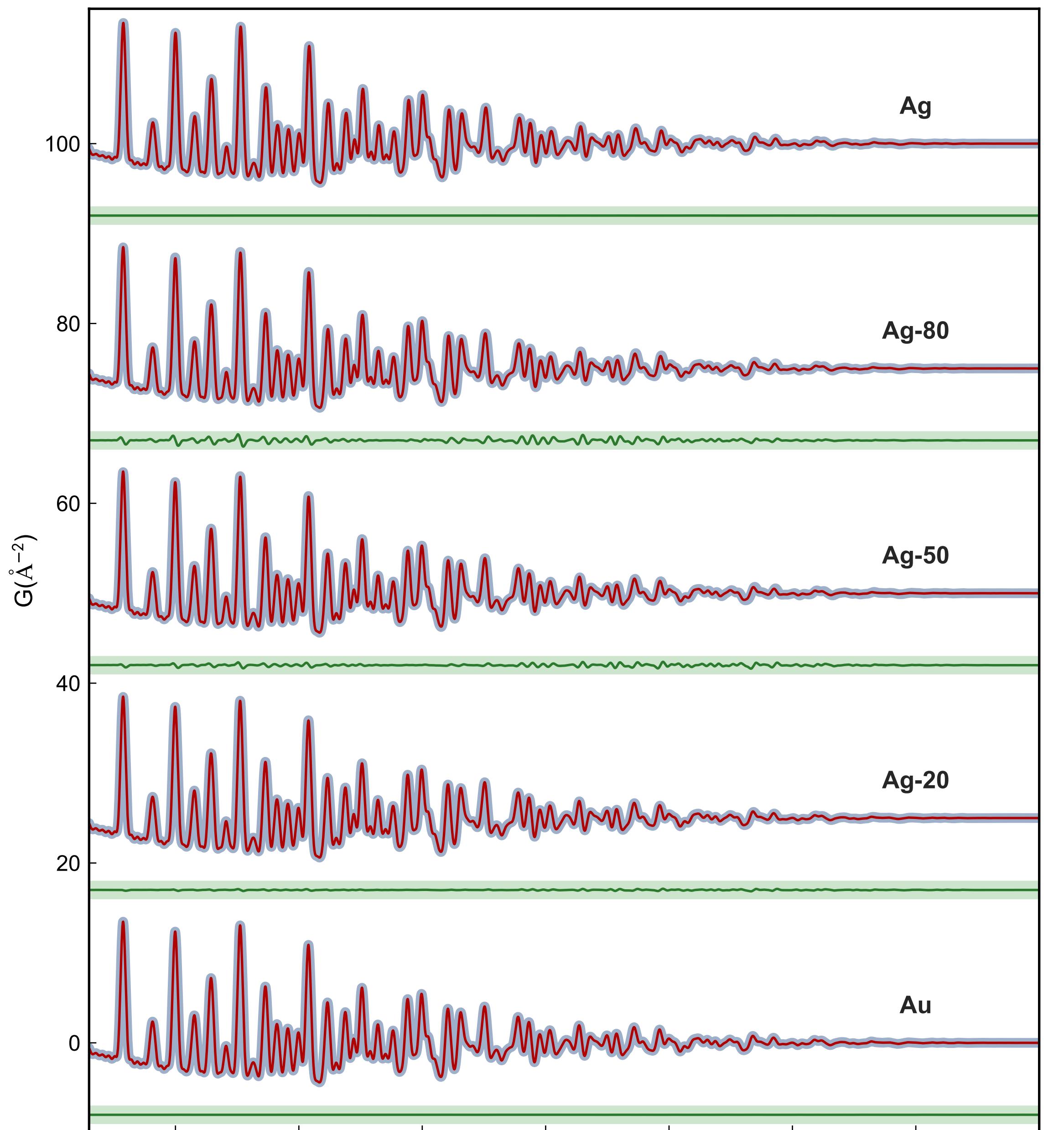
Pearson Correlation Map : FitResiduals – AgAu – FCCAlloy

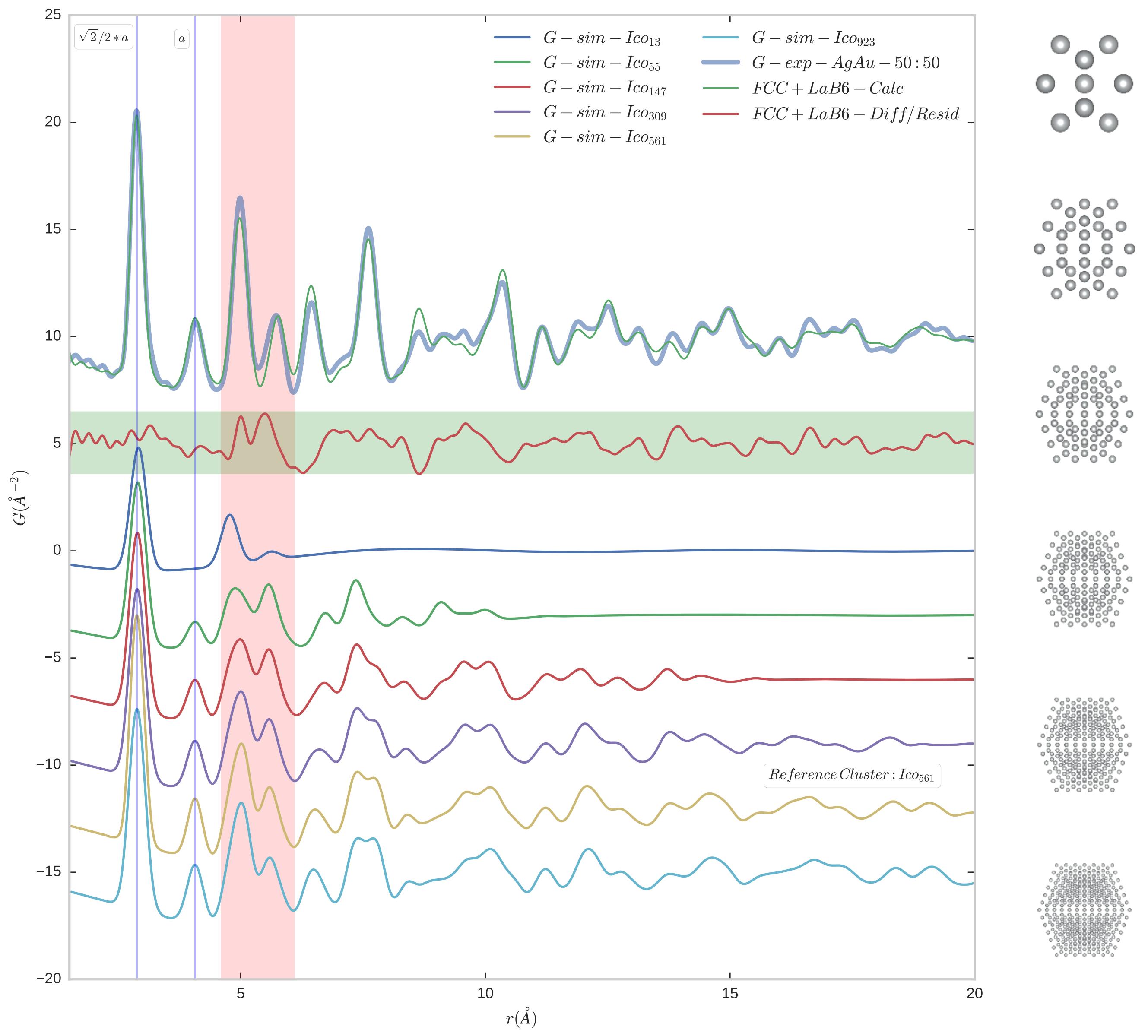


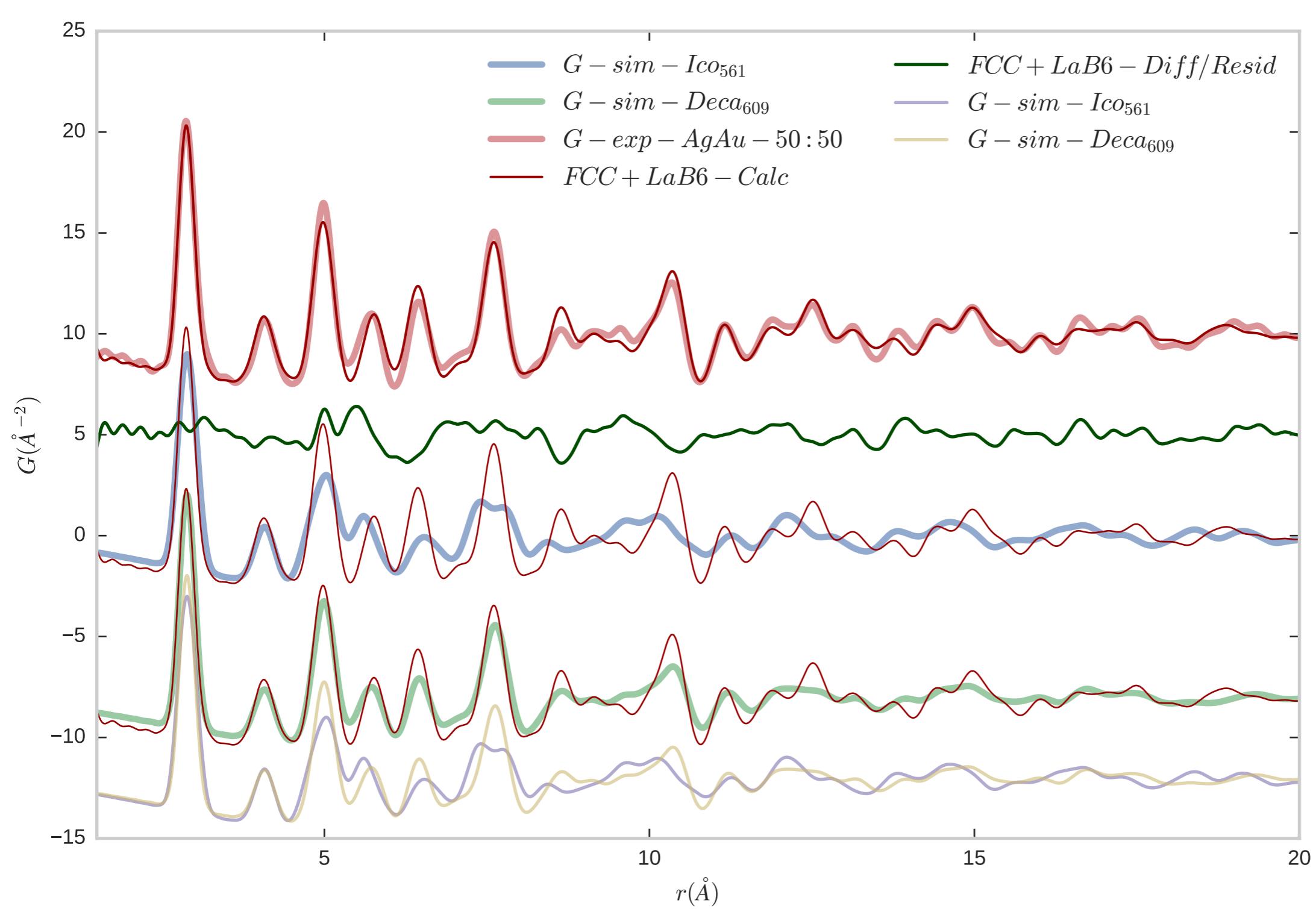




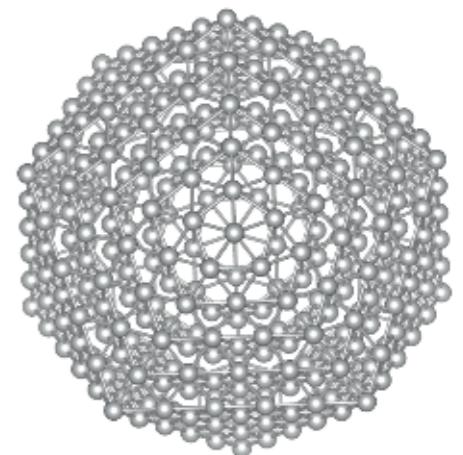




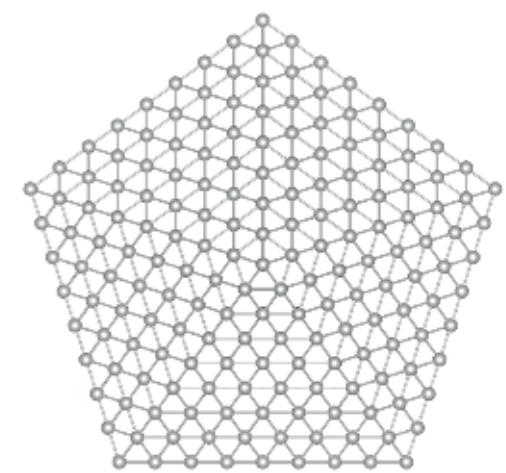




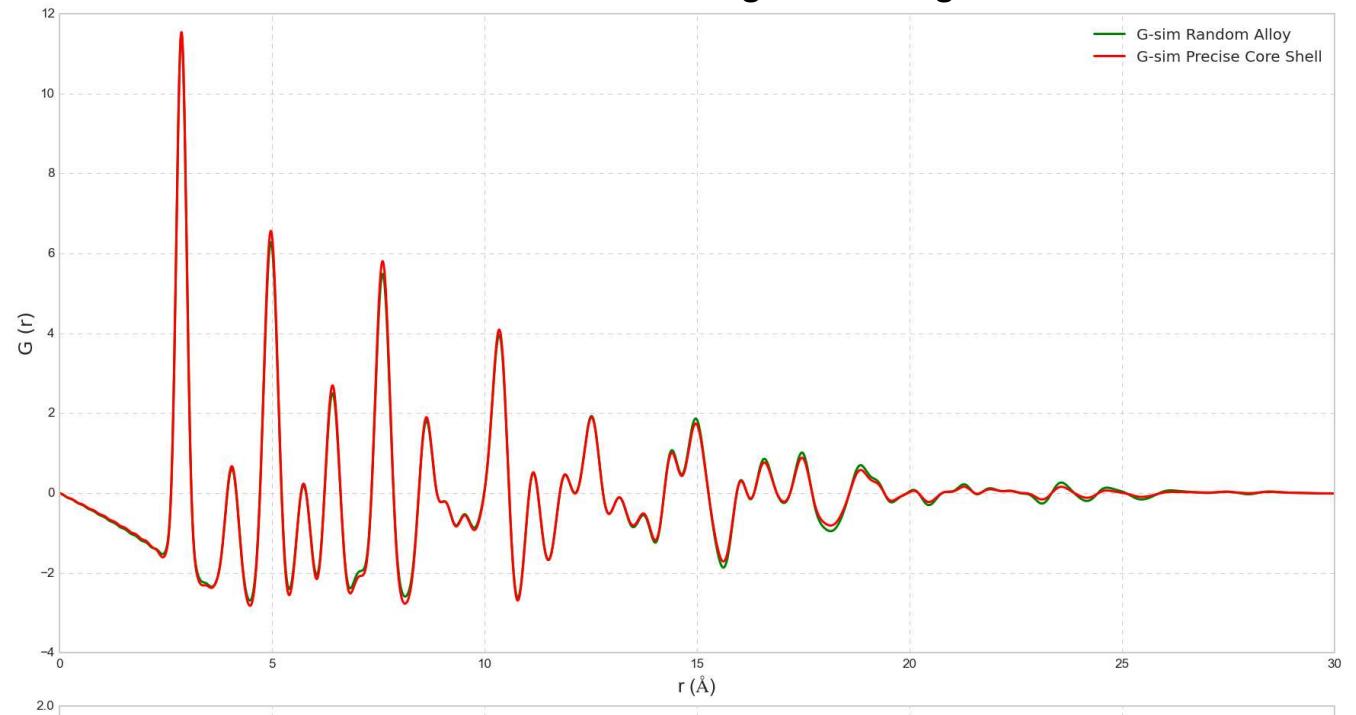
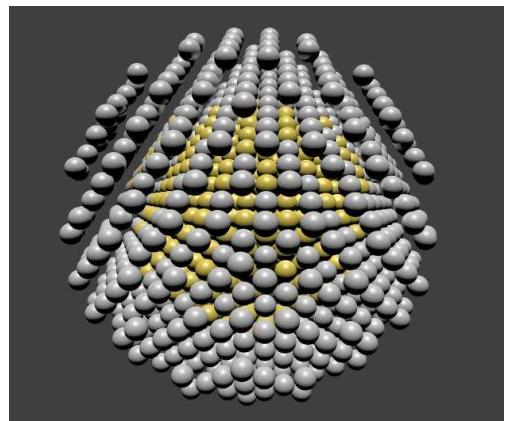
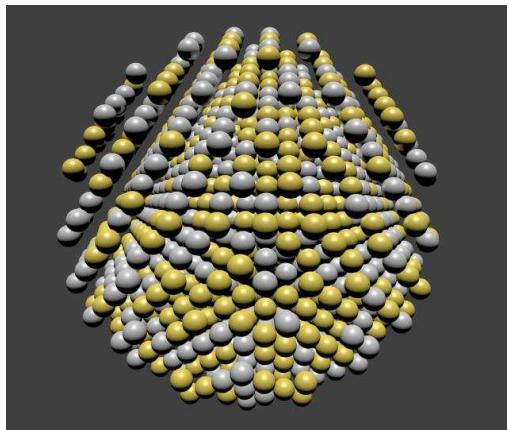
$Ico_{561}$



$Marks_{609} - 9 - 9 - 9$



## Discrete NP Modeling: A Learning Exercise



$$Volume_{core} = \frac{4}{3}\pi r_{Au}^3$$

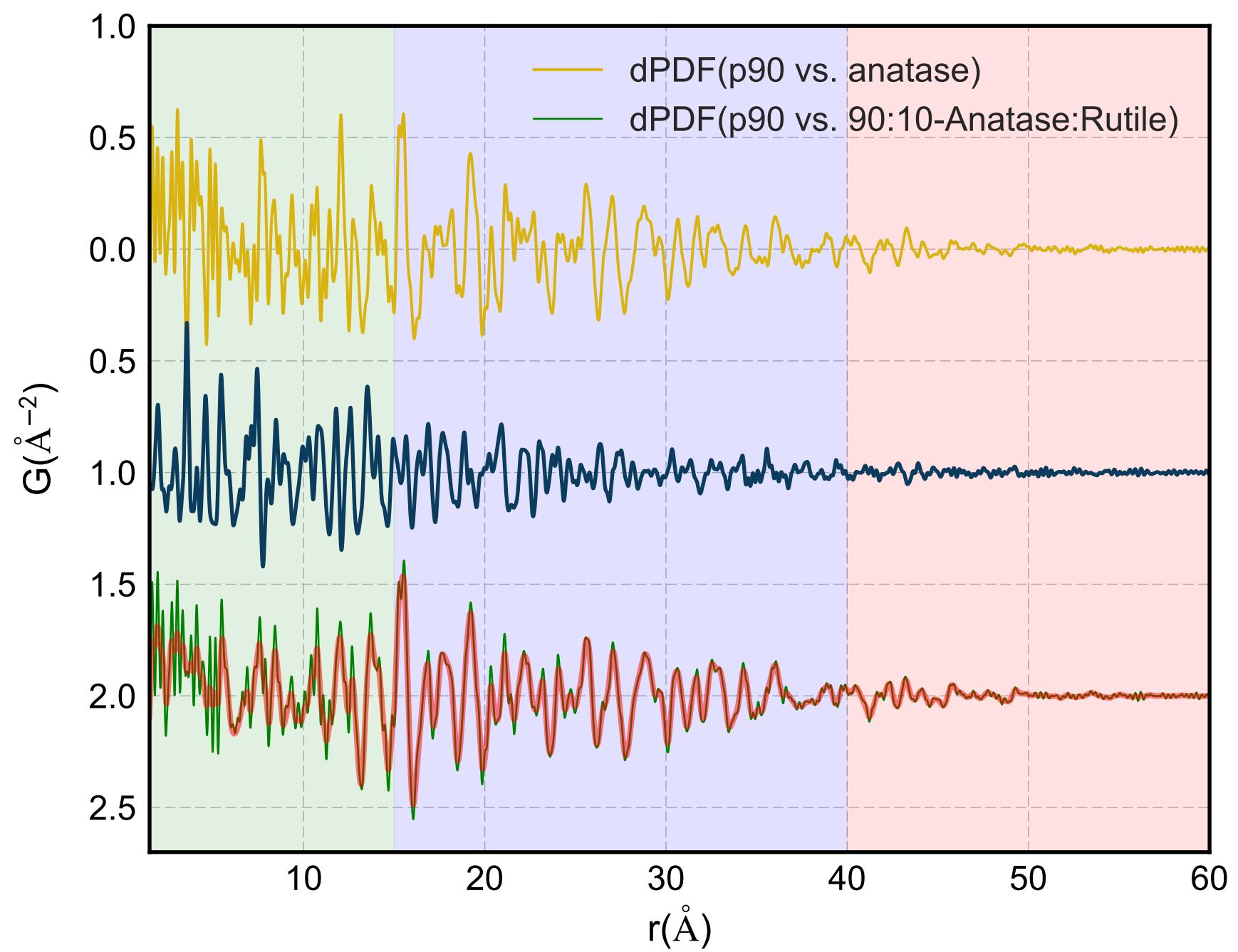
$$Volume_{shell} = \frac{4}{3}\pi(R_{Ag}^3 - r_{Au}^3)$$

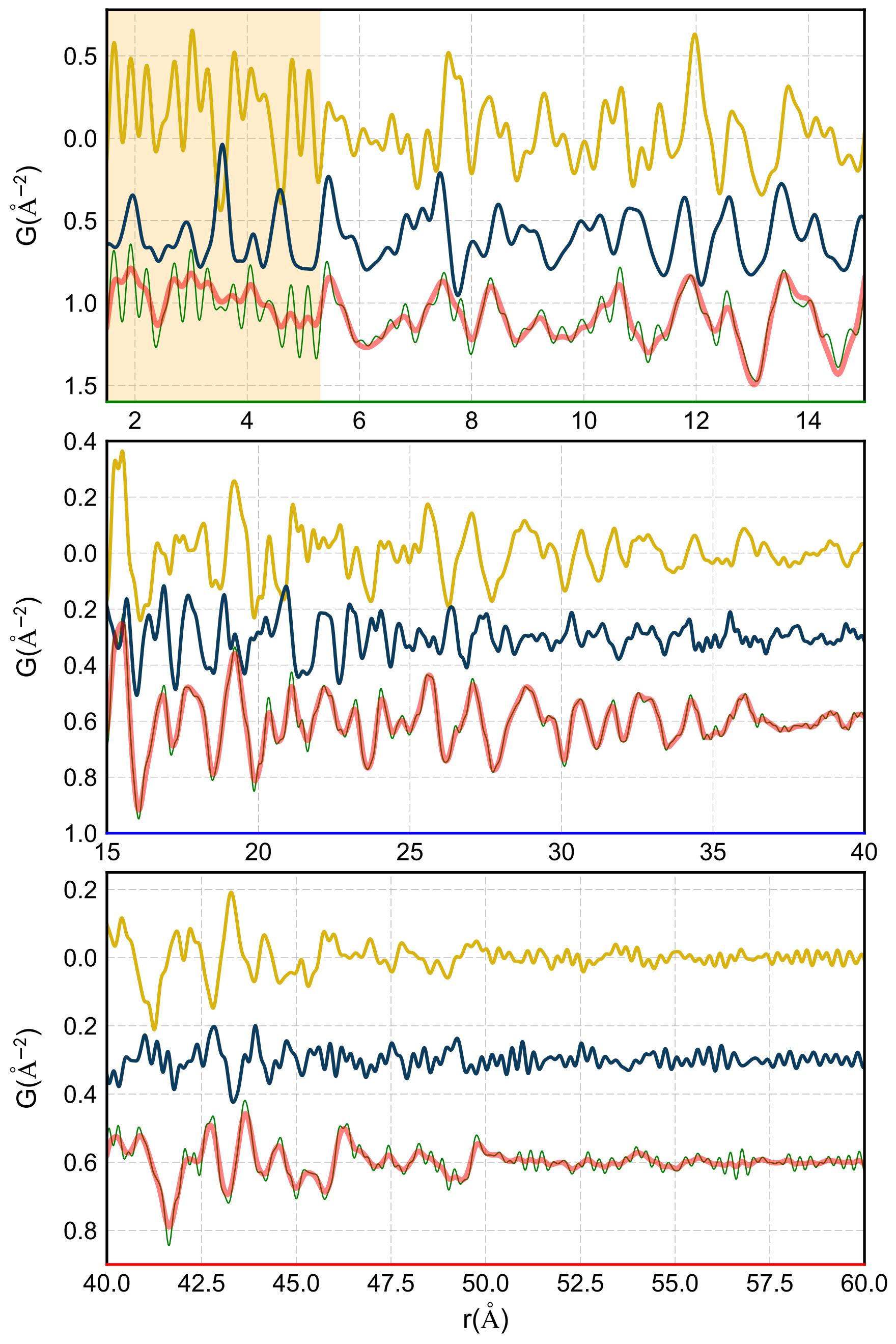
$$\frac{Volume_{core}}{Volume_{shell}} = Composition = \frac{r_{Au}^3}{R_{Ag}^3 - r_{Au}^3}$$

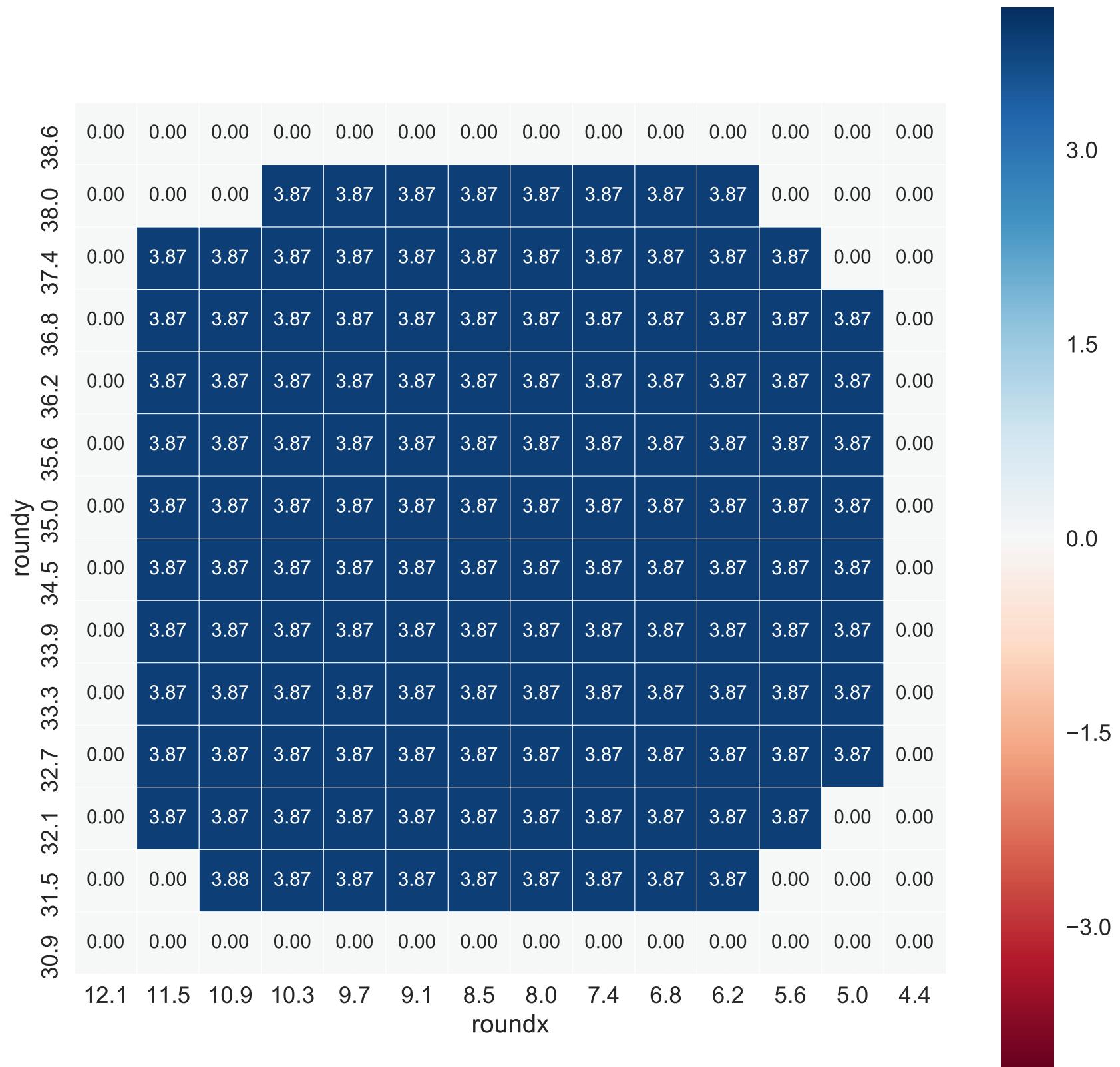
$$R_{NP} \equiv R_{Ag}$$

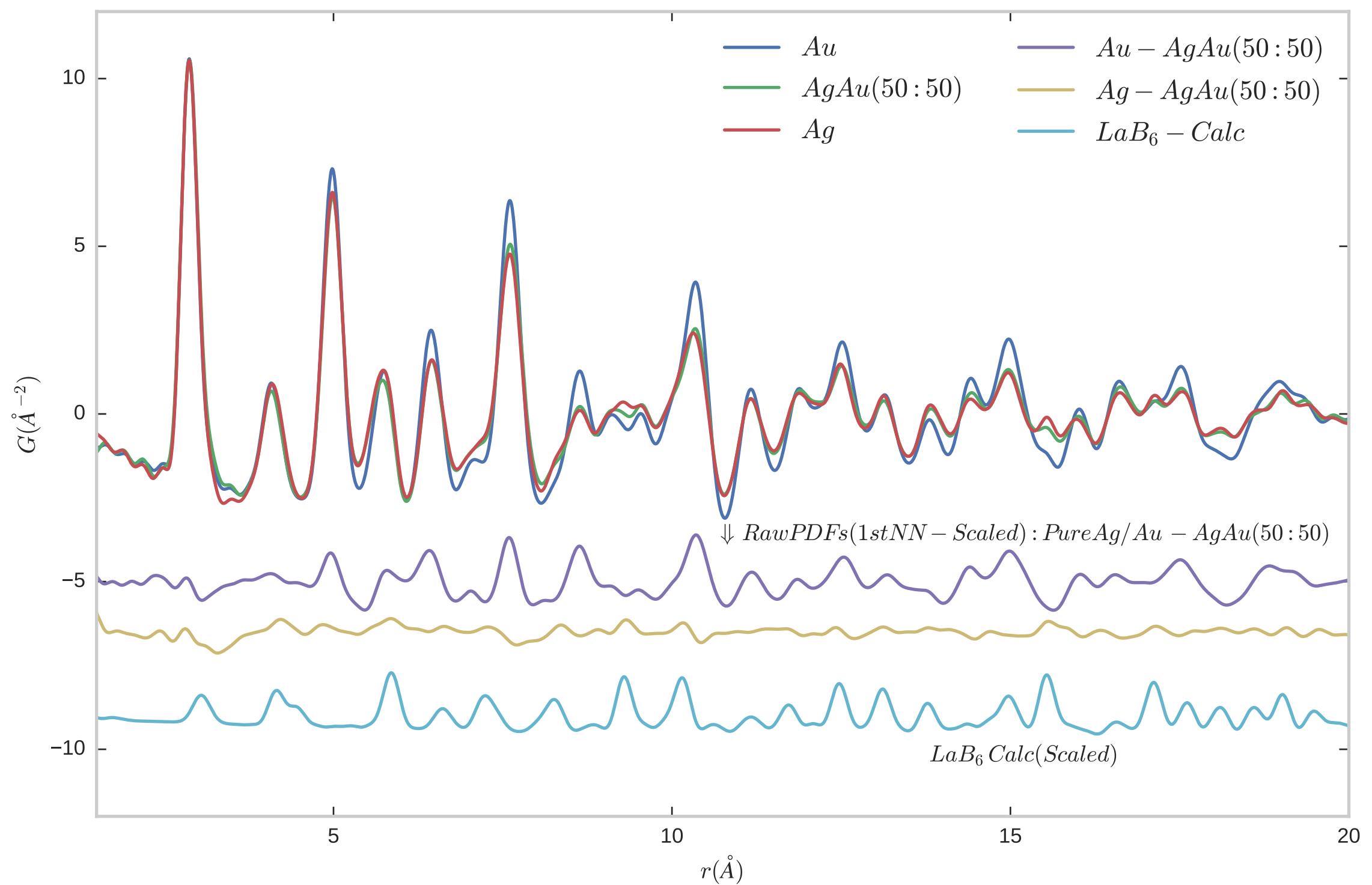
$$R_{Shell} \equiv R_{NP} - R_{Au} = R_{NP} - r_{Au}$$

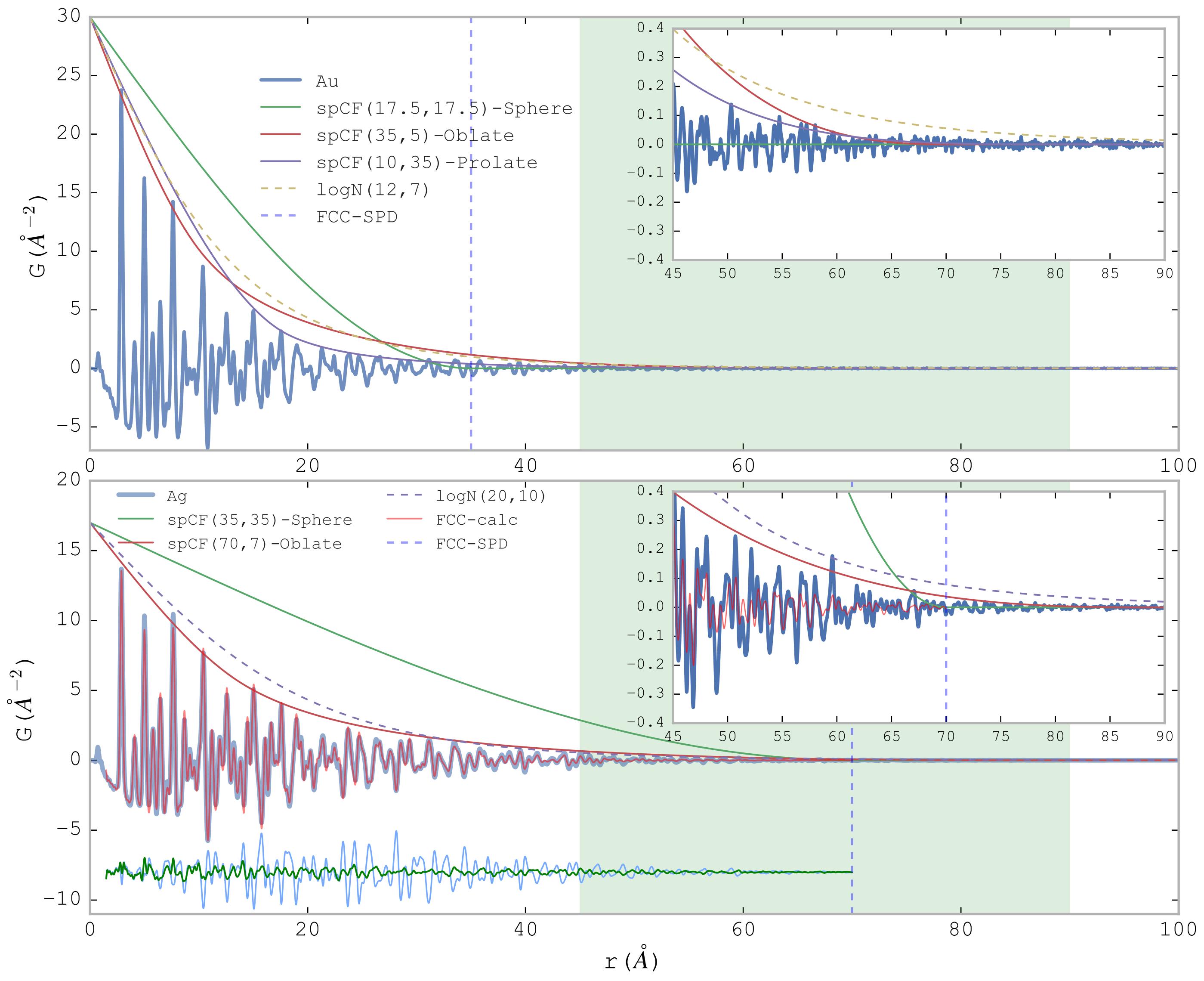
$$r_{Au} = \left( \frac{R_{Ag} \times Composition}{1 + Composition} \right)^{\frac{1}{3}} = \left( \frac{R_{NP} \times Composition}{1 + Composition} \right)^{\frac{1}{3}}$$



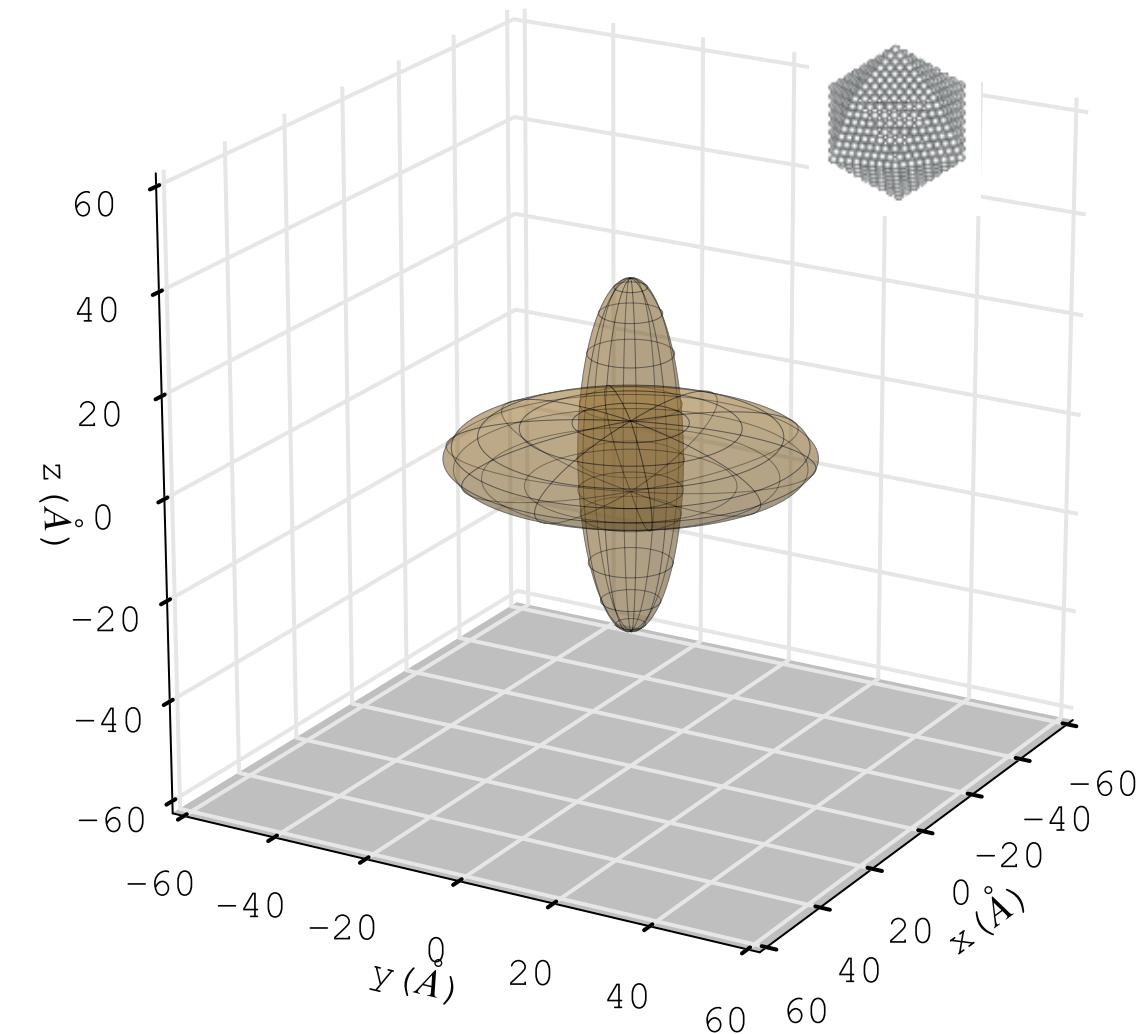




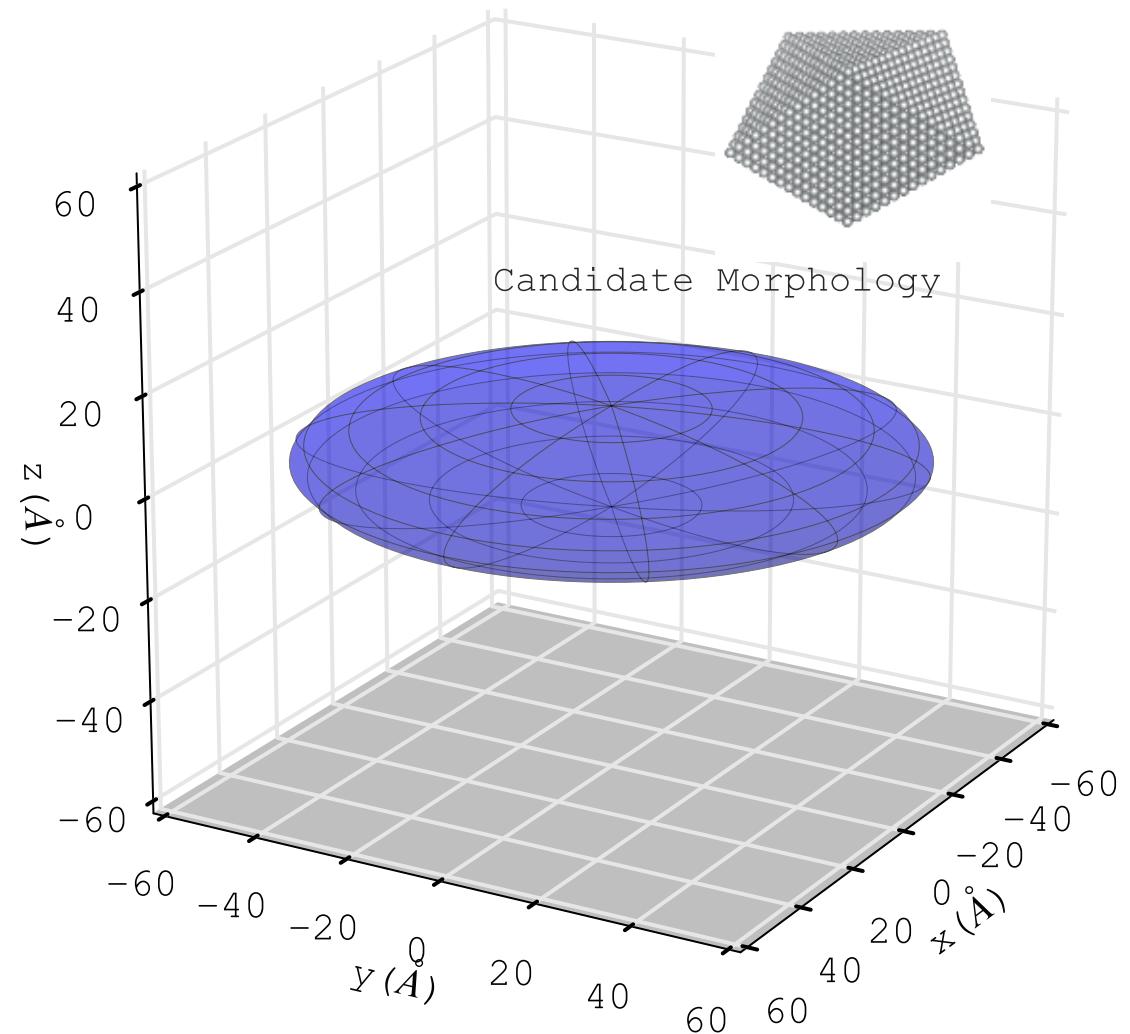


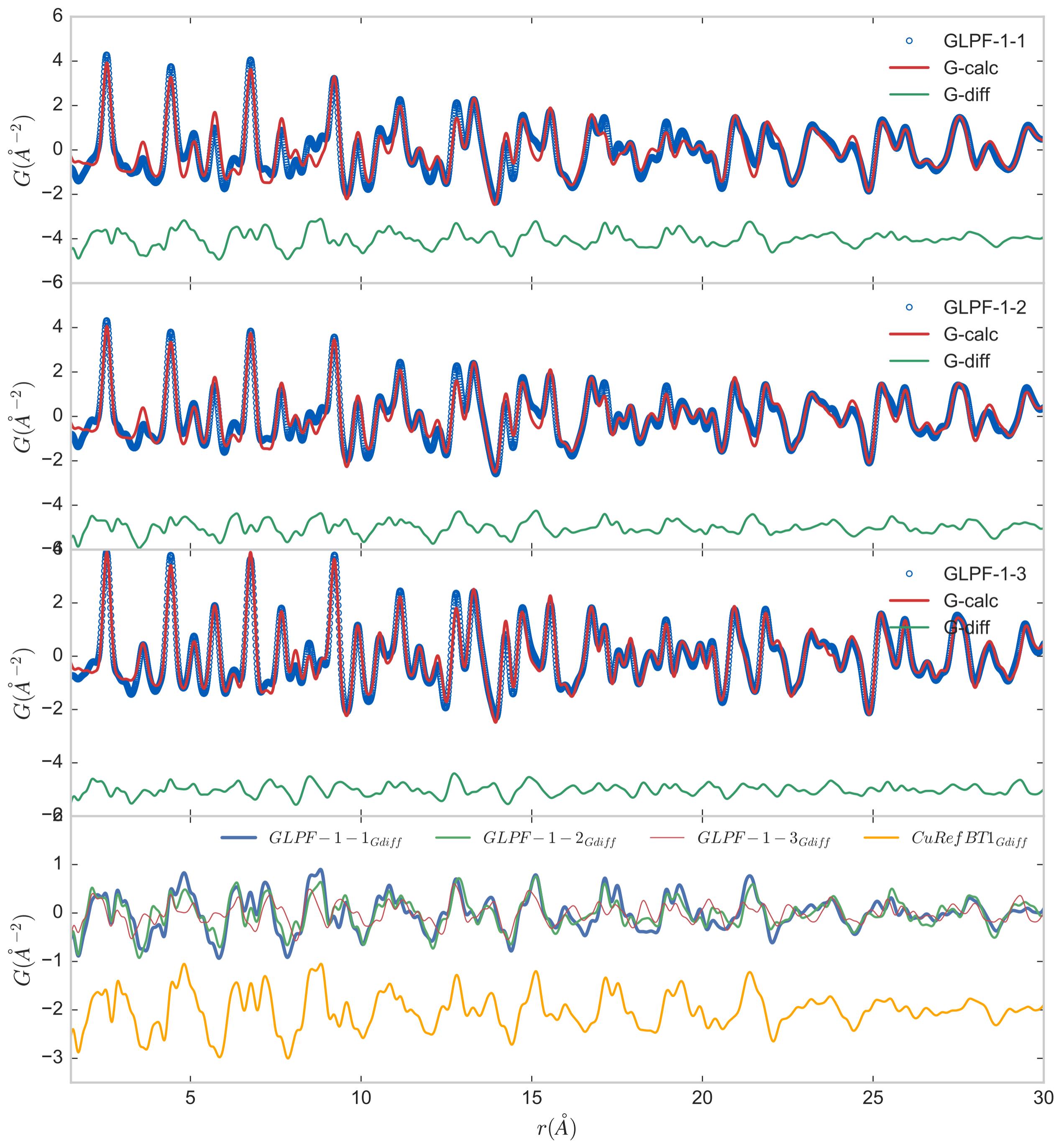


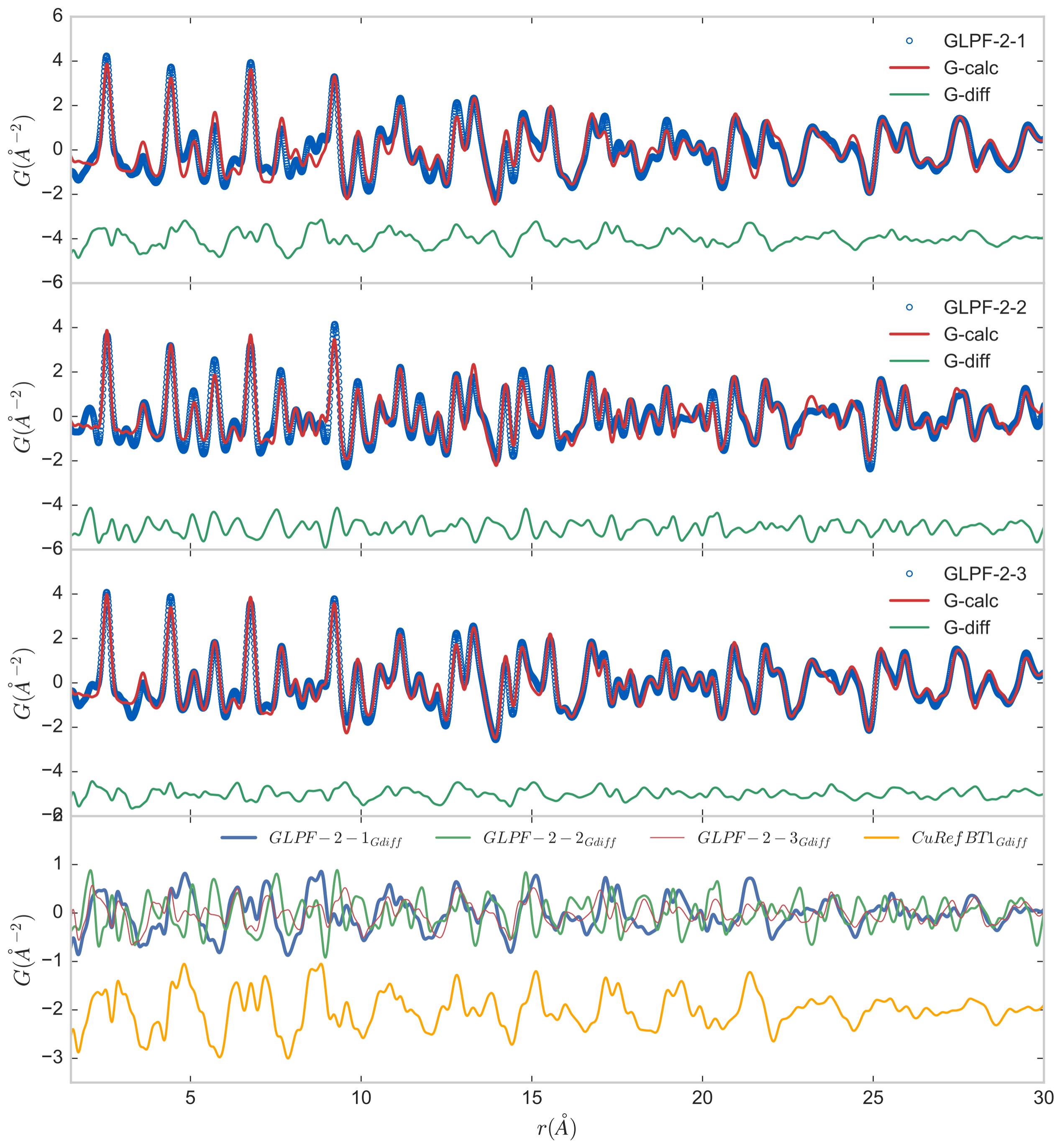
Au Form Factor (Oblate+Prolate)

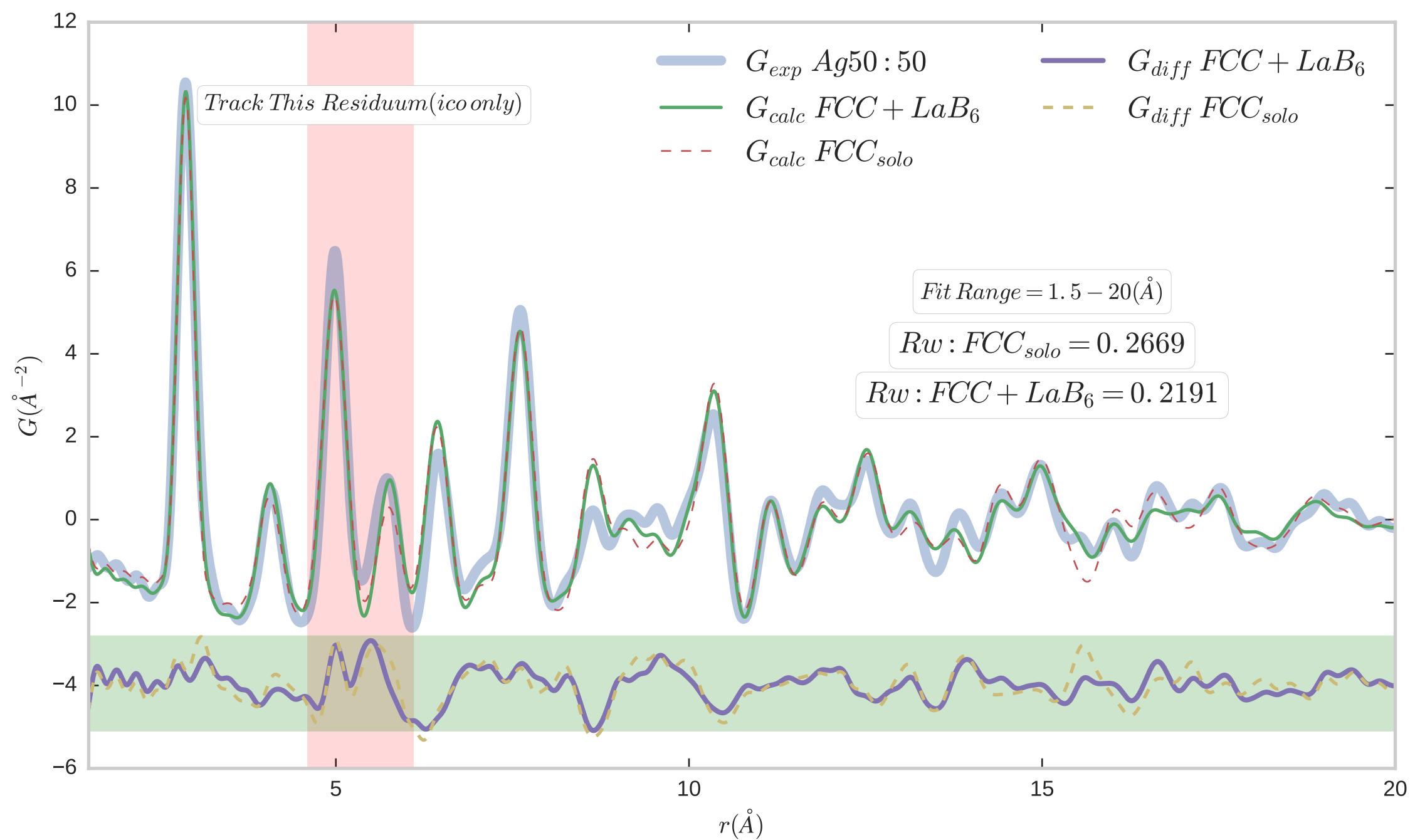


Ag Form Factor (Oblate)

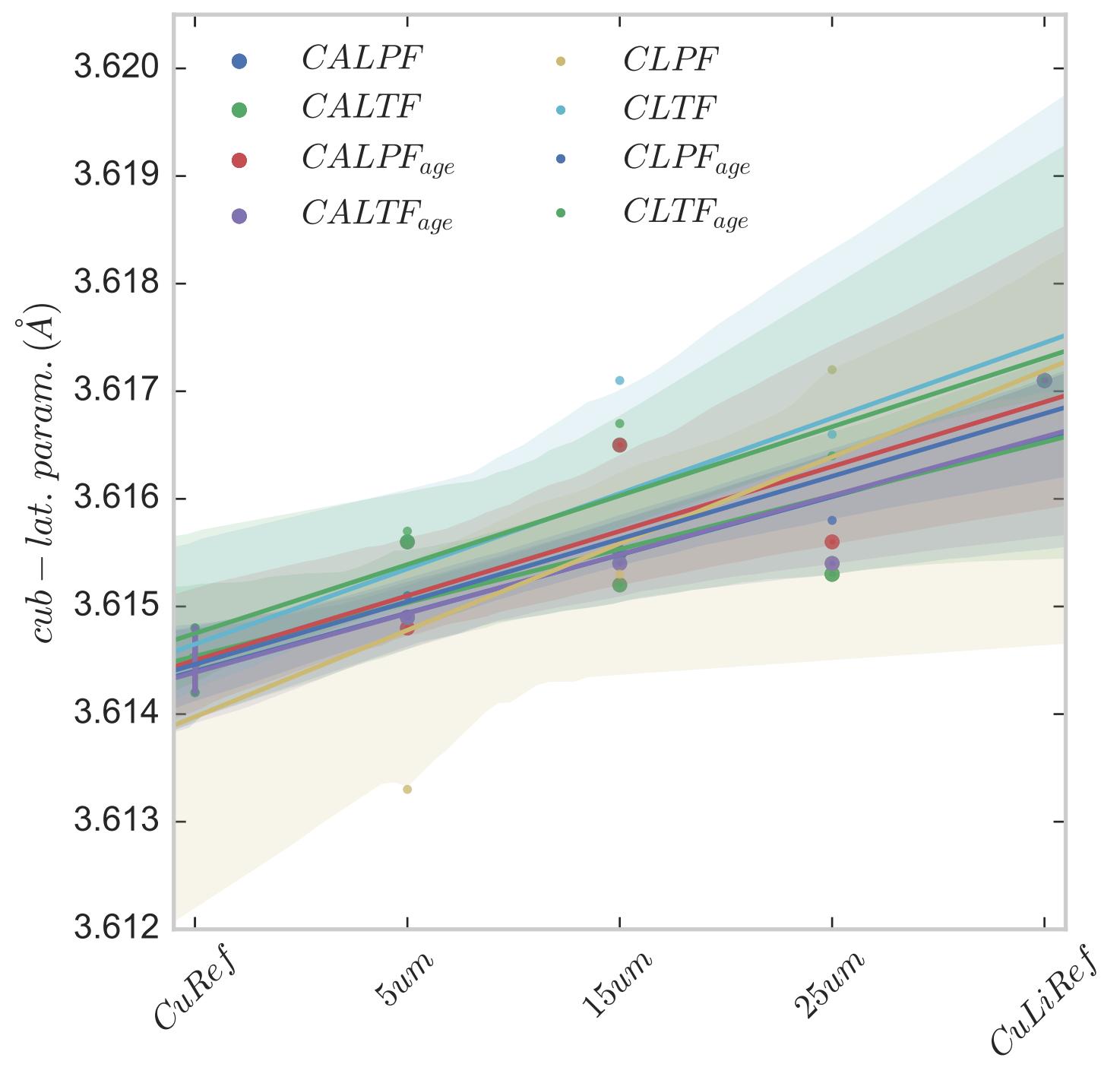


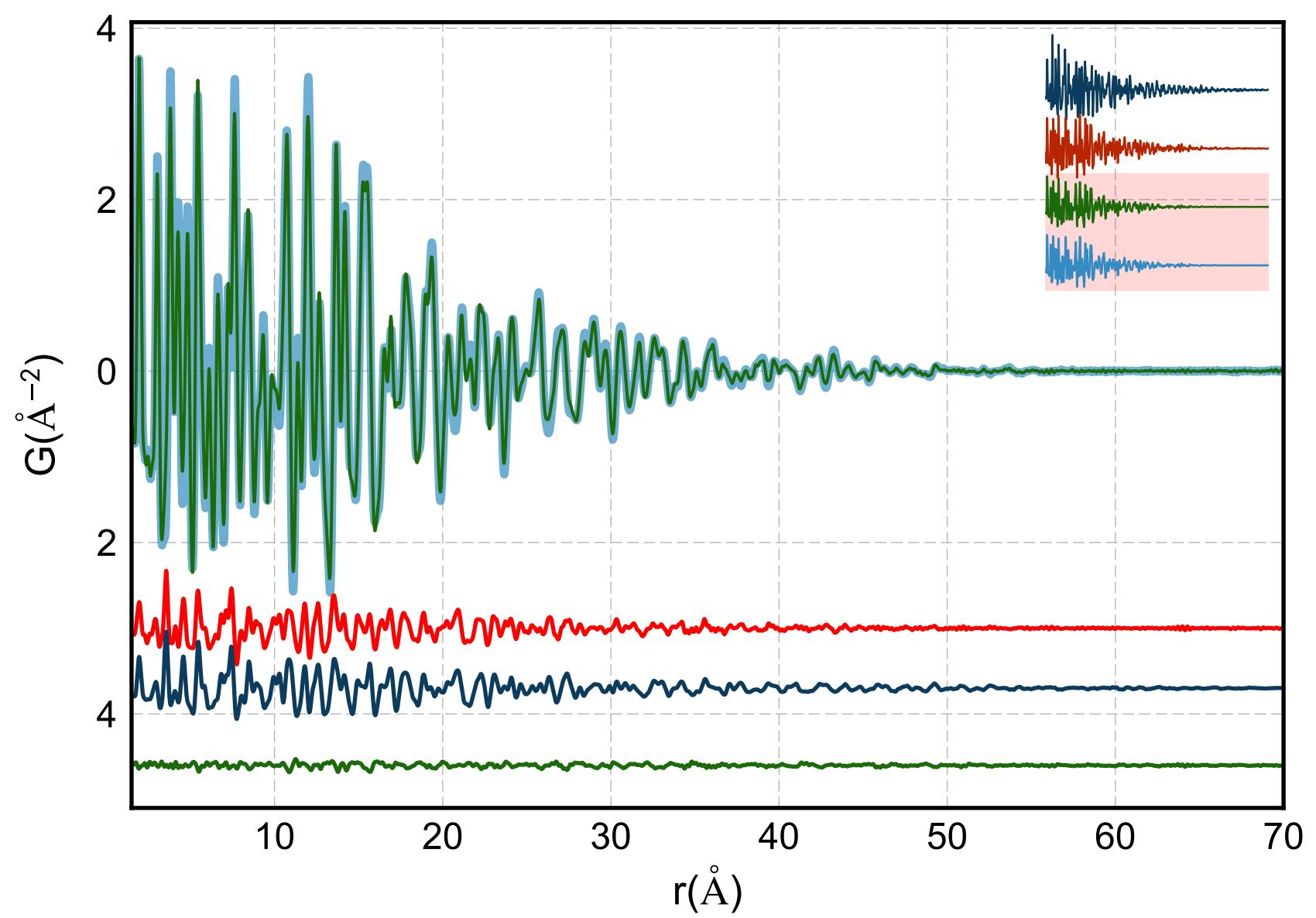


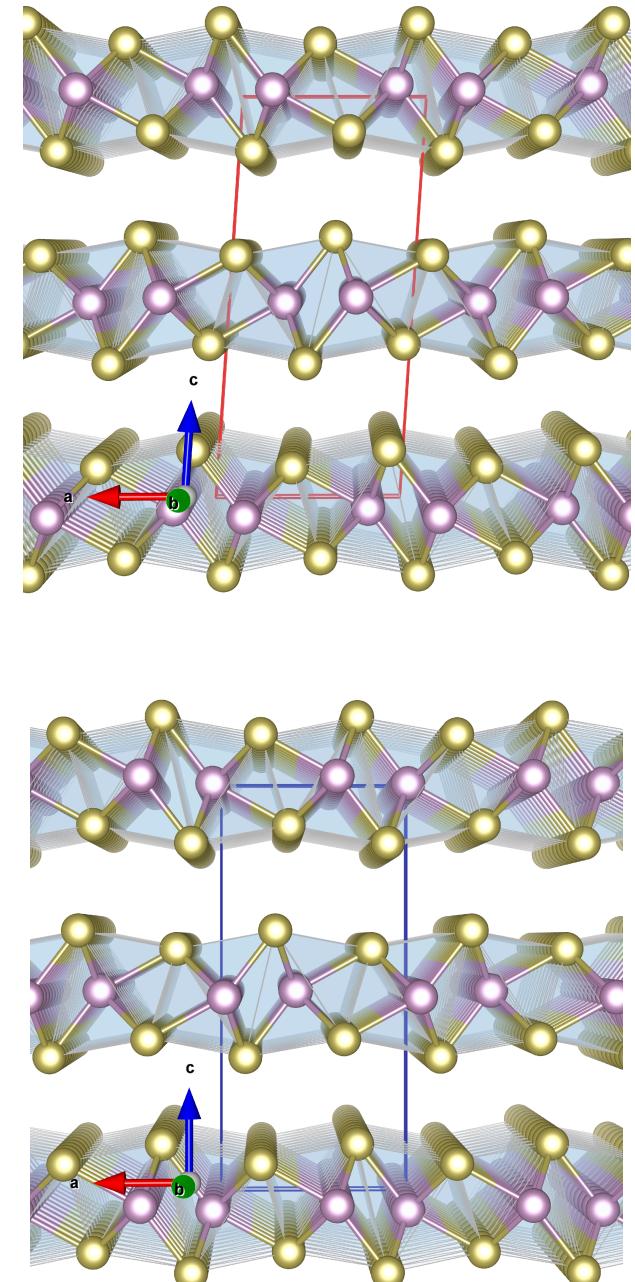
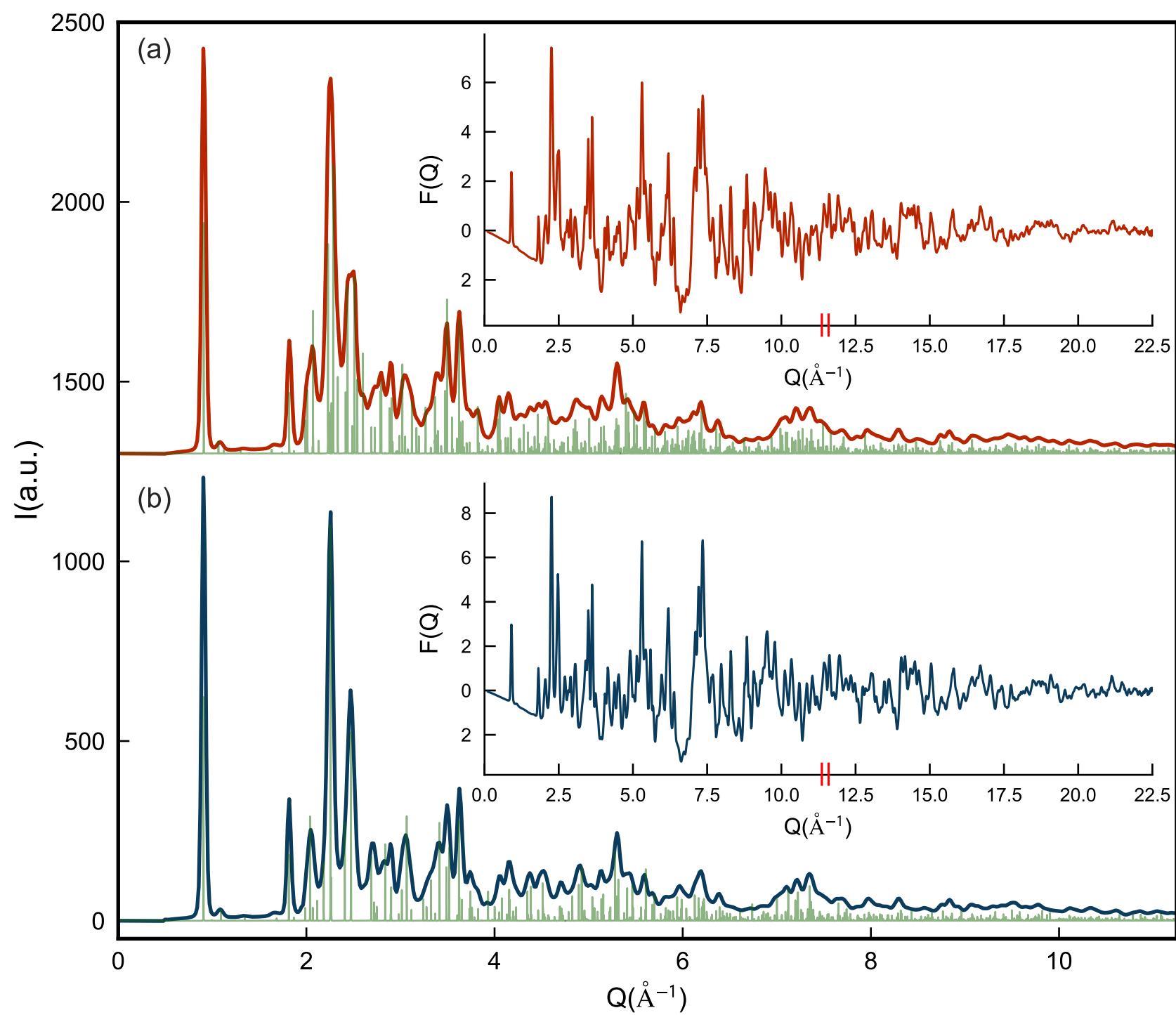


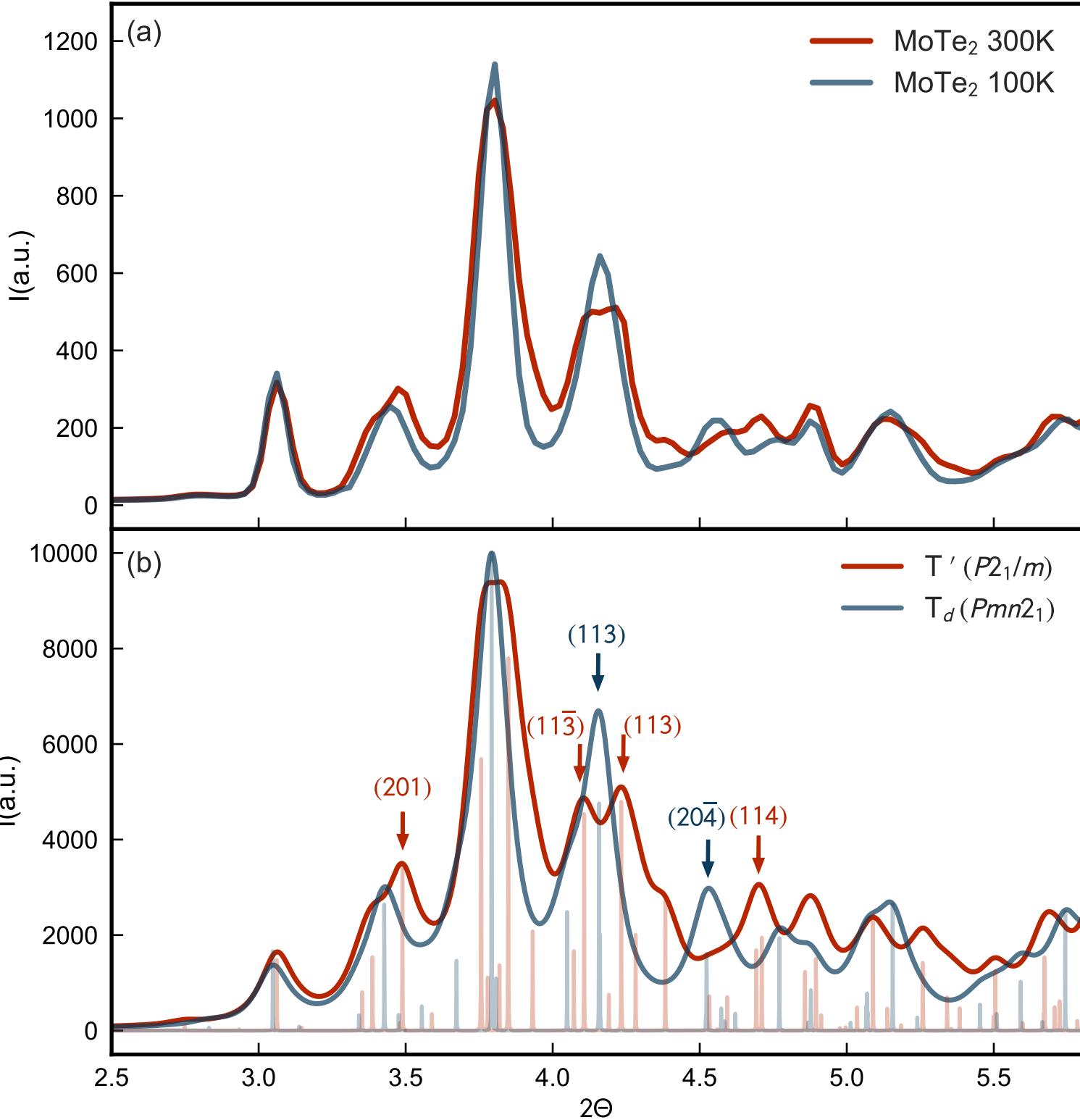


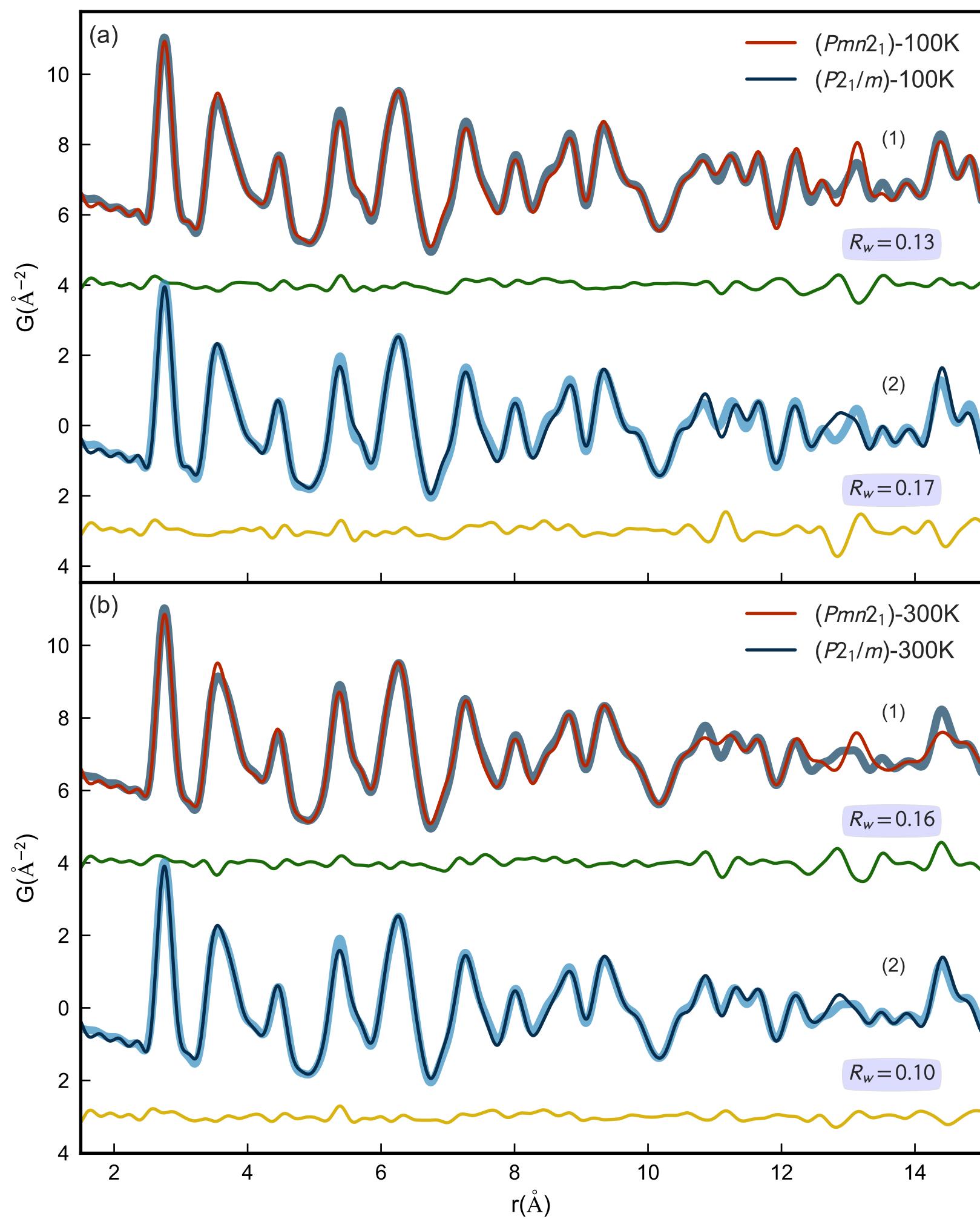


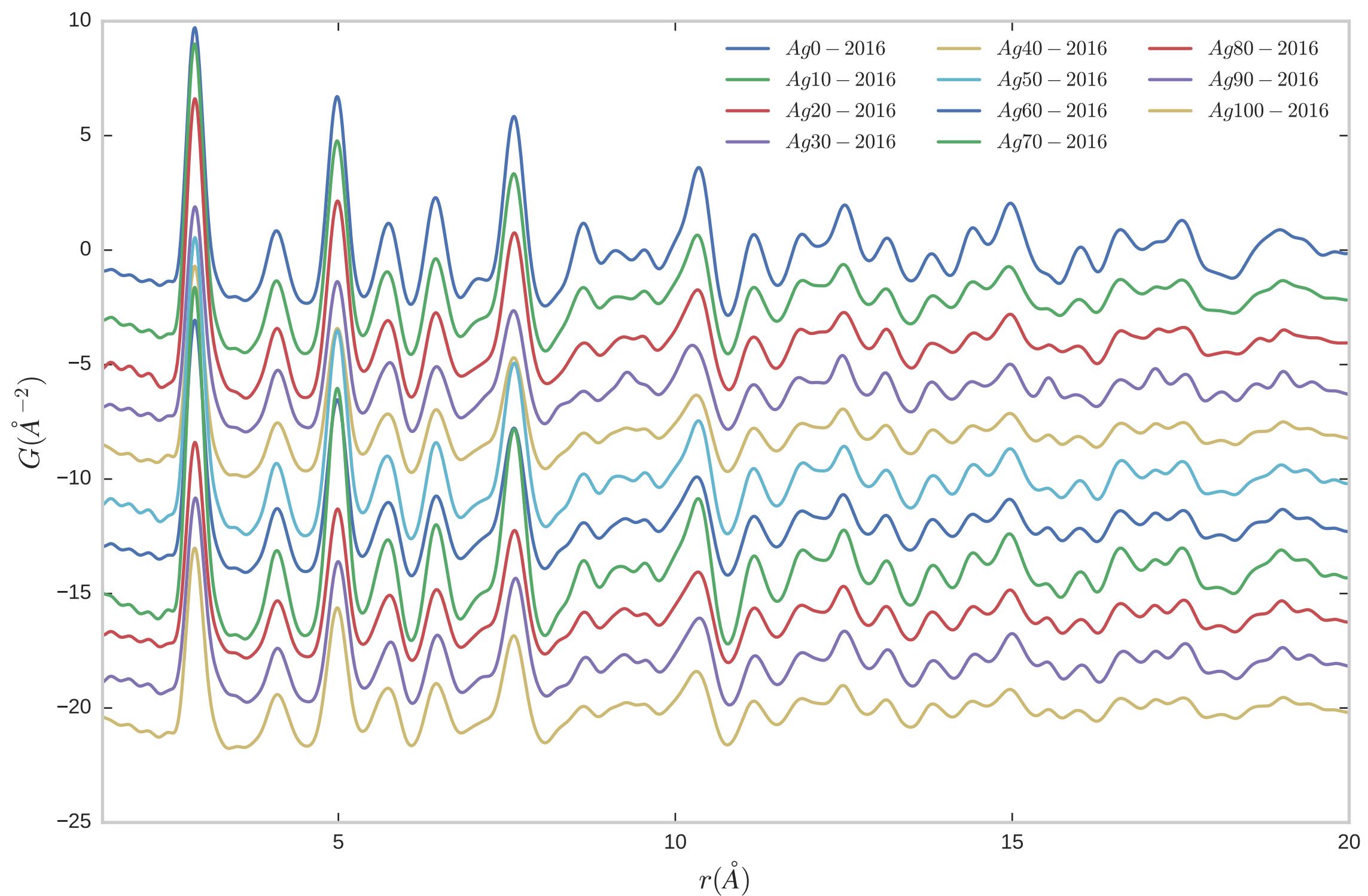


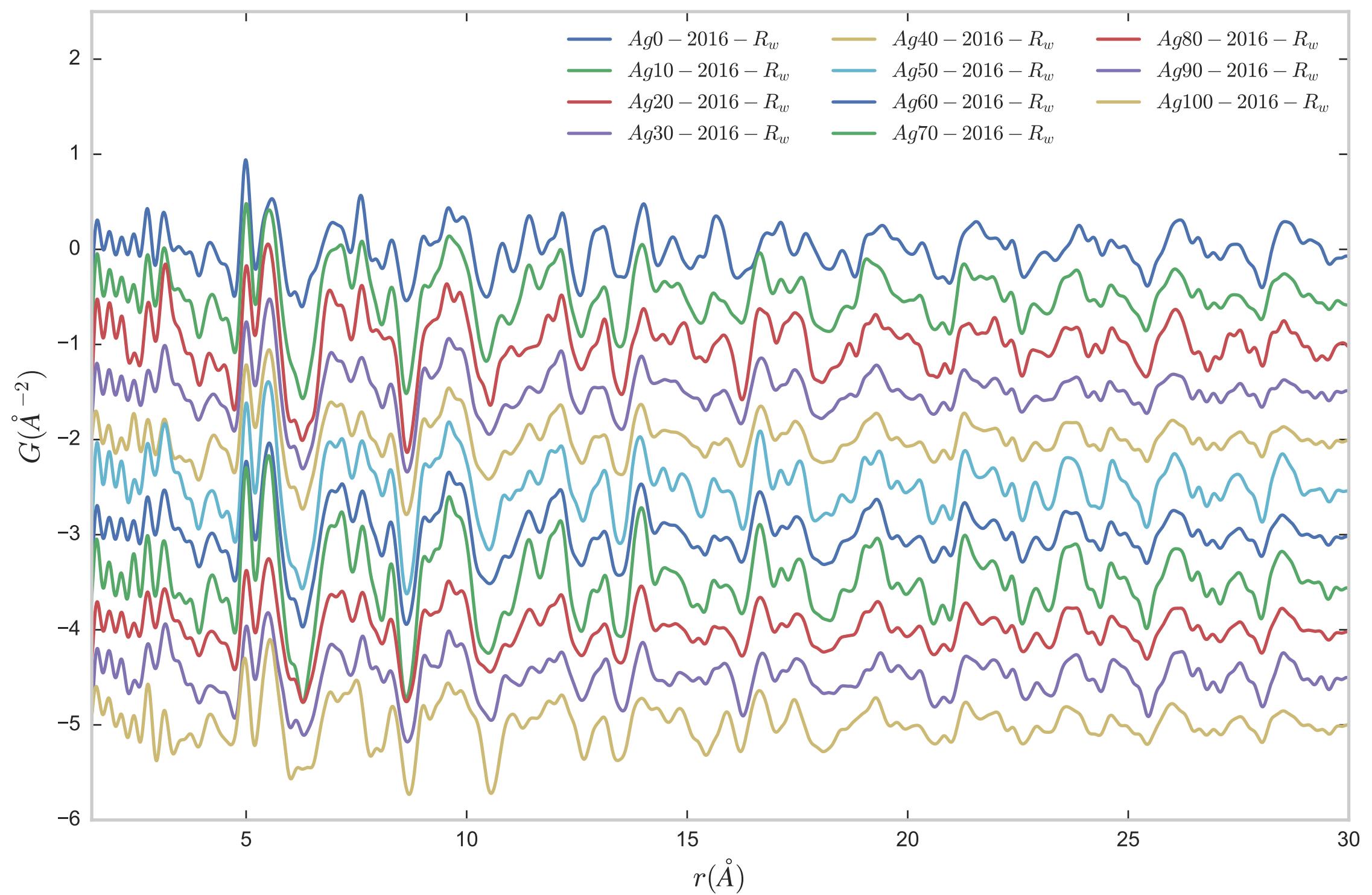


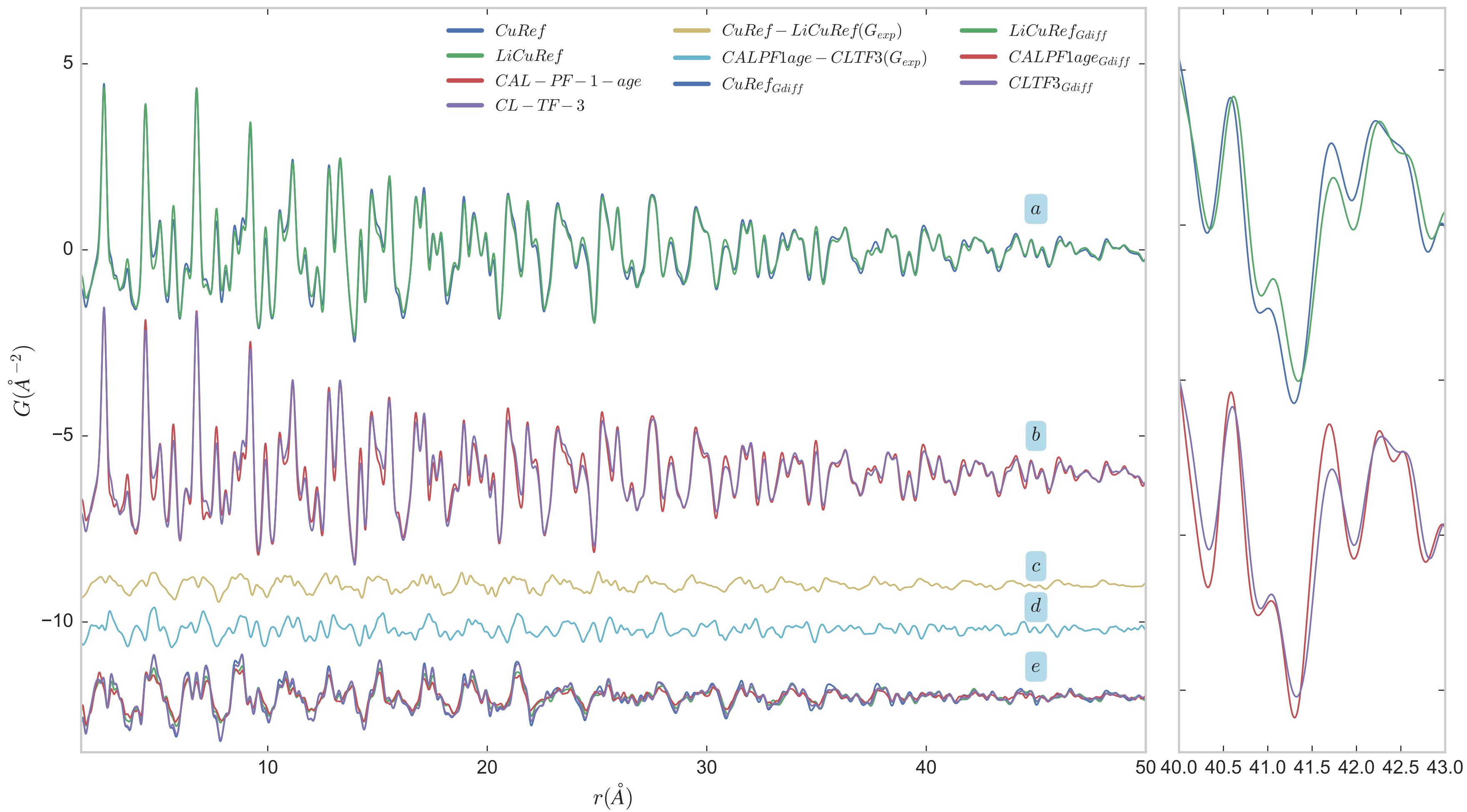


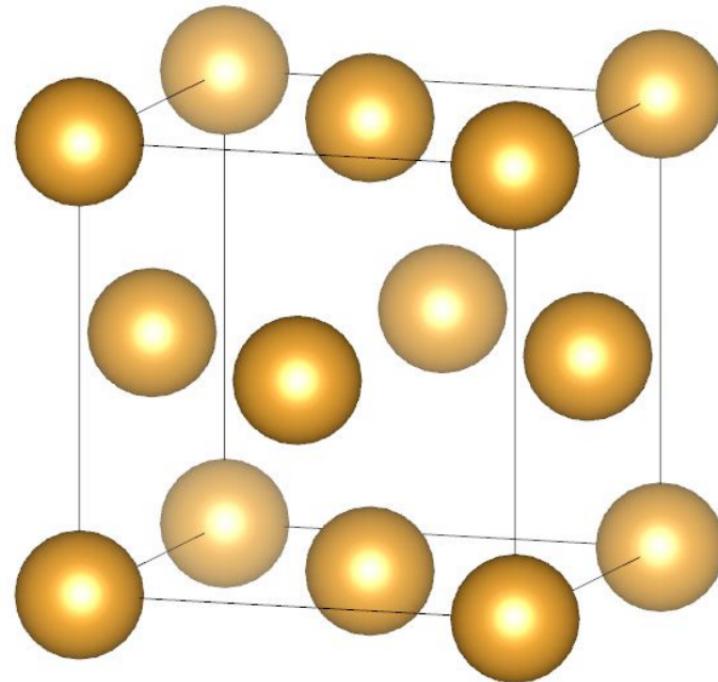




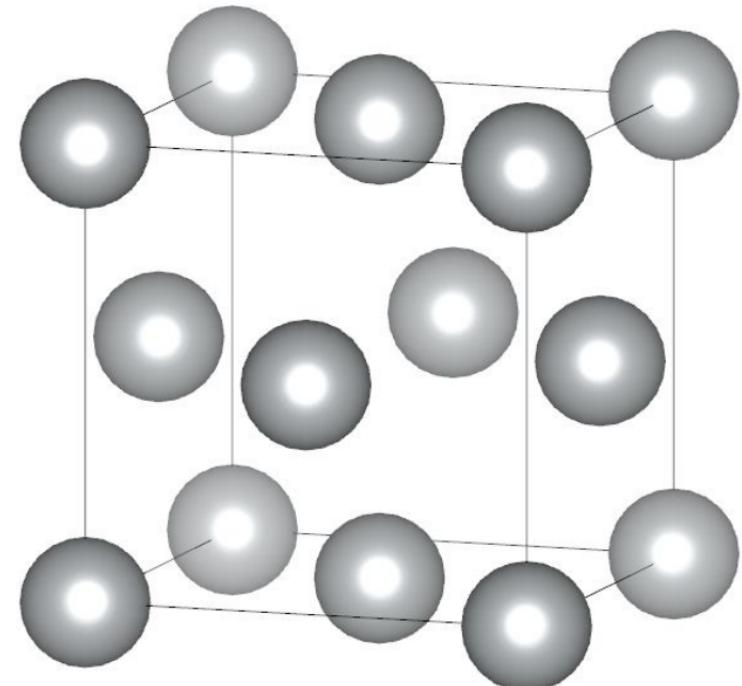
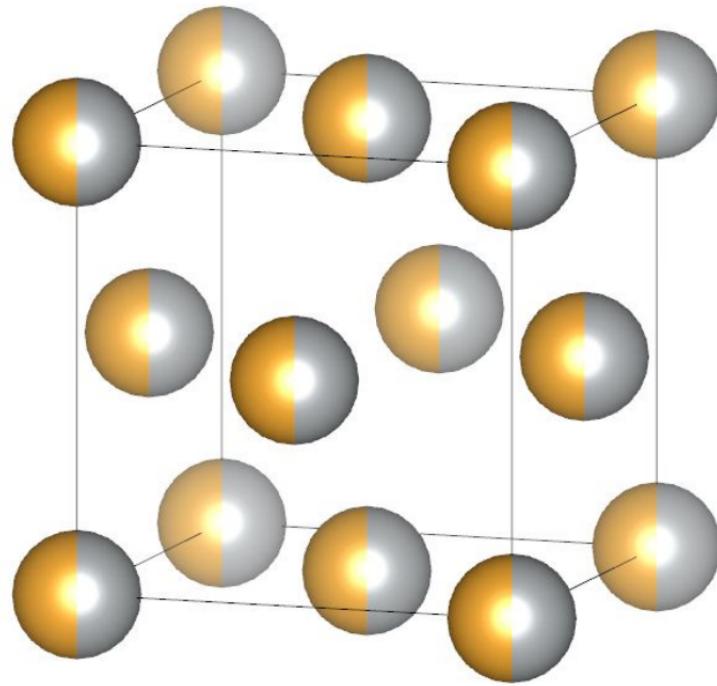




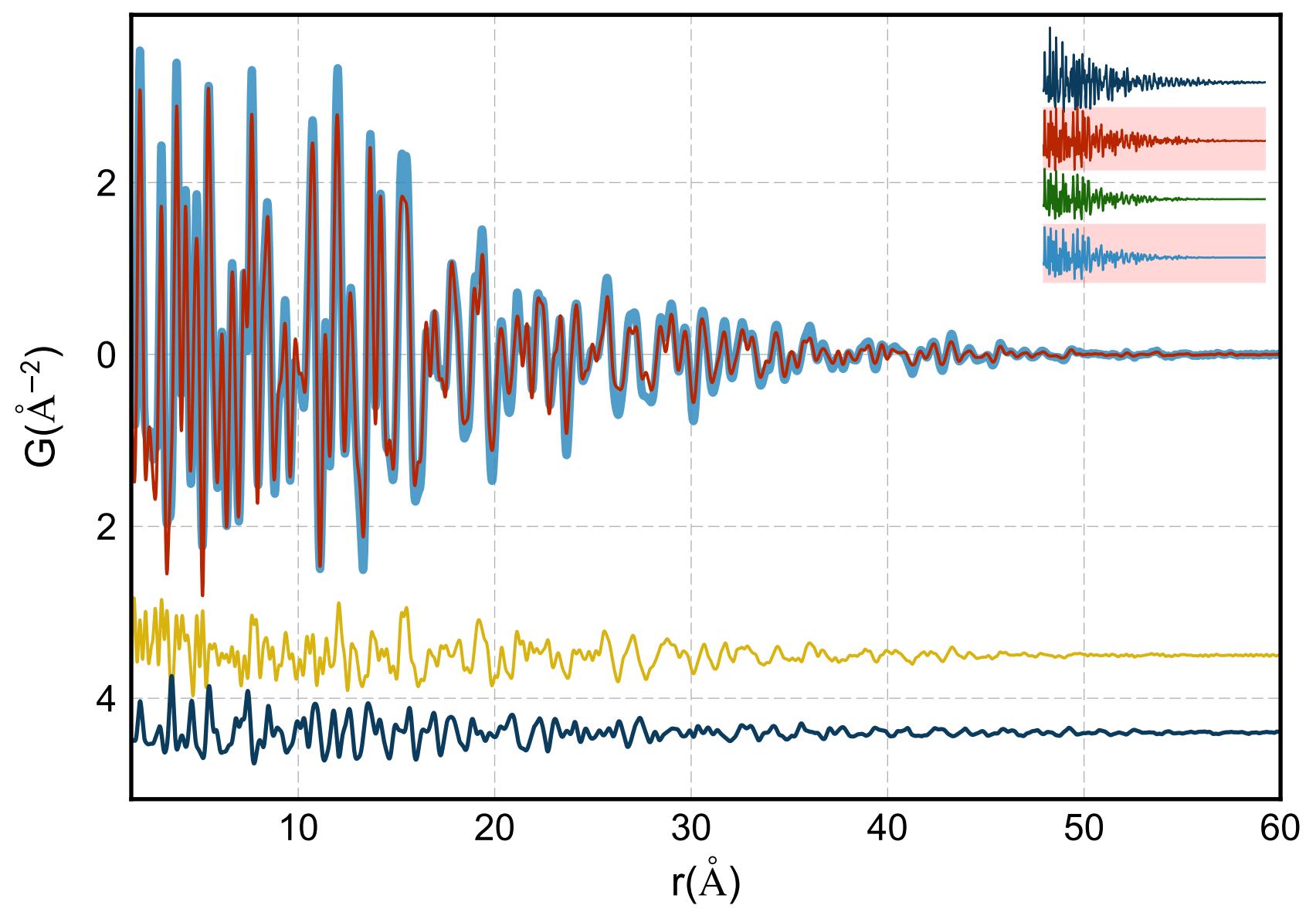


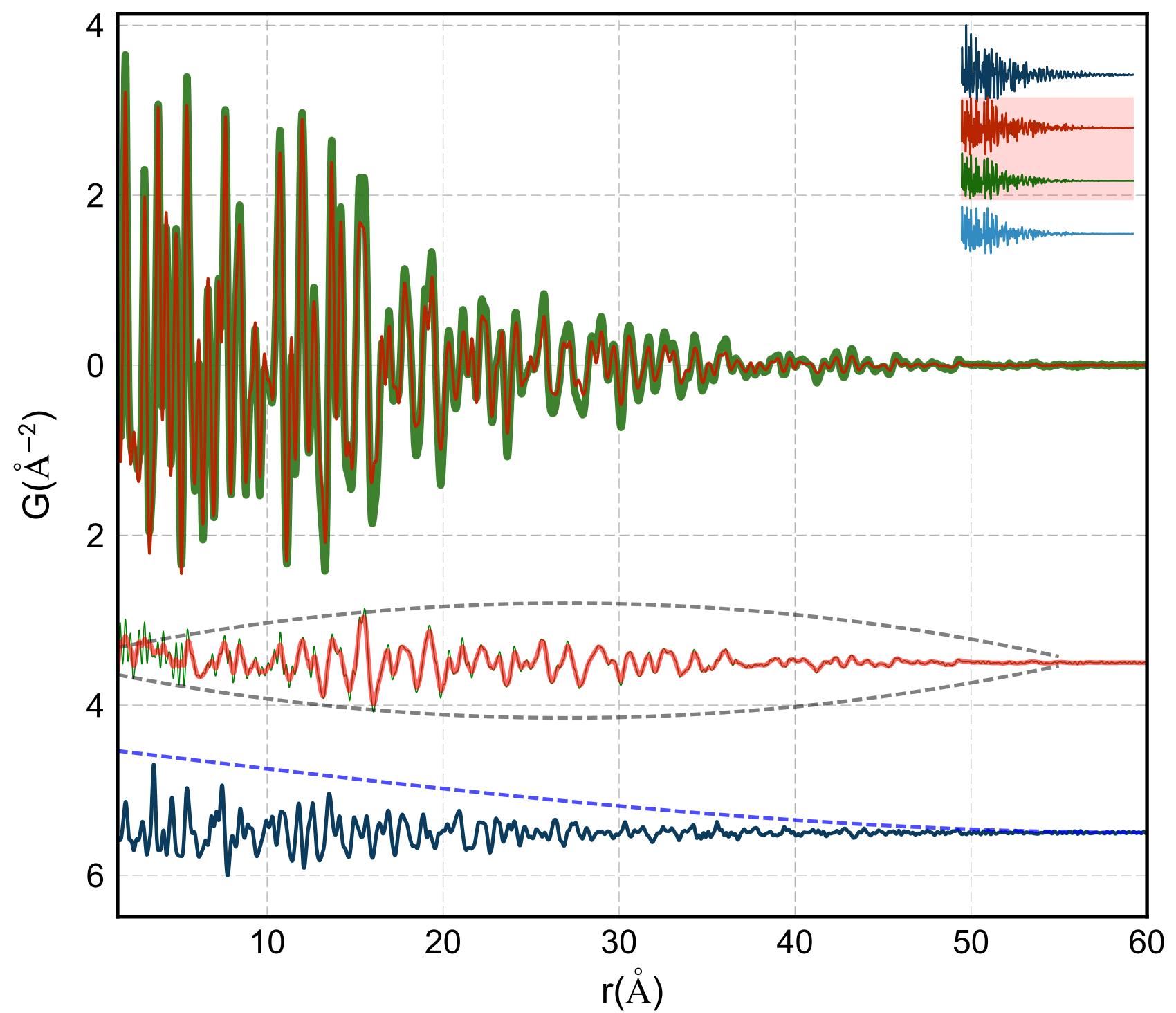


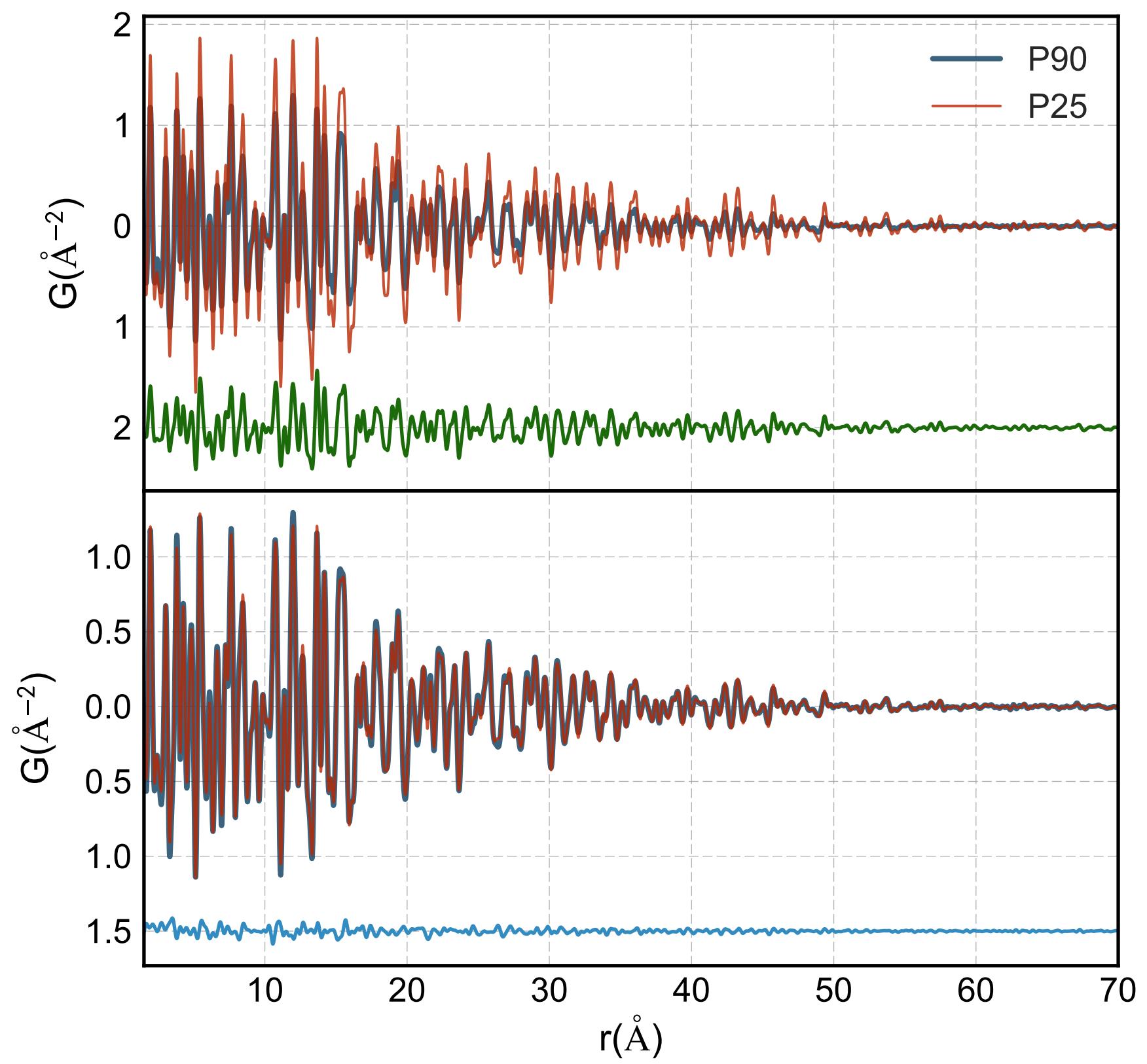
*Au*

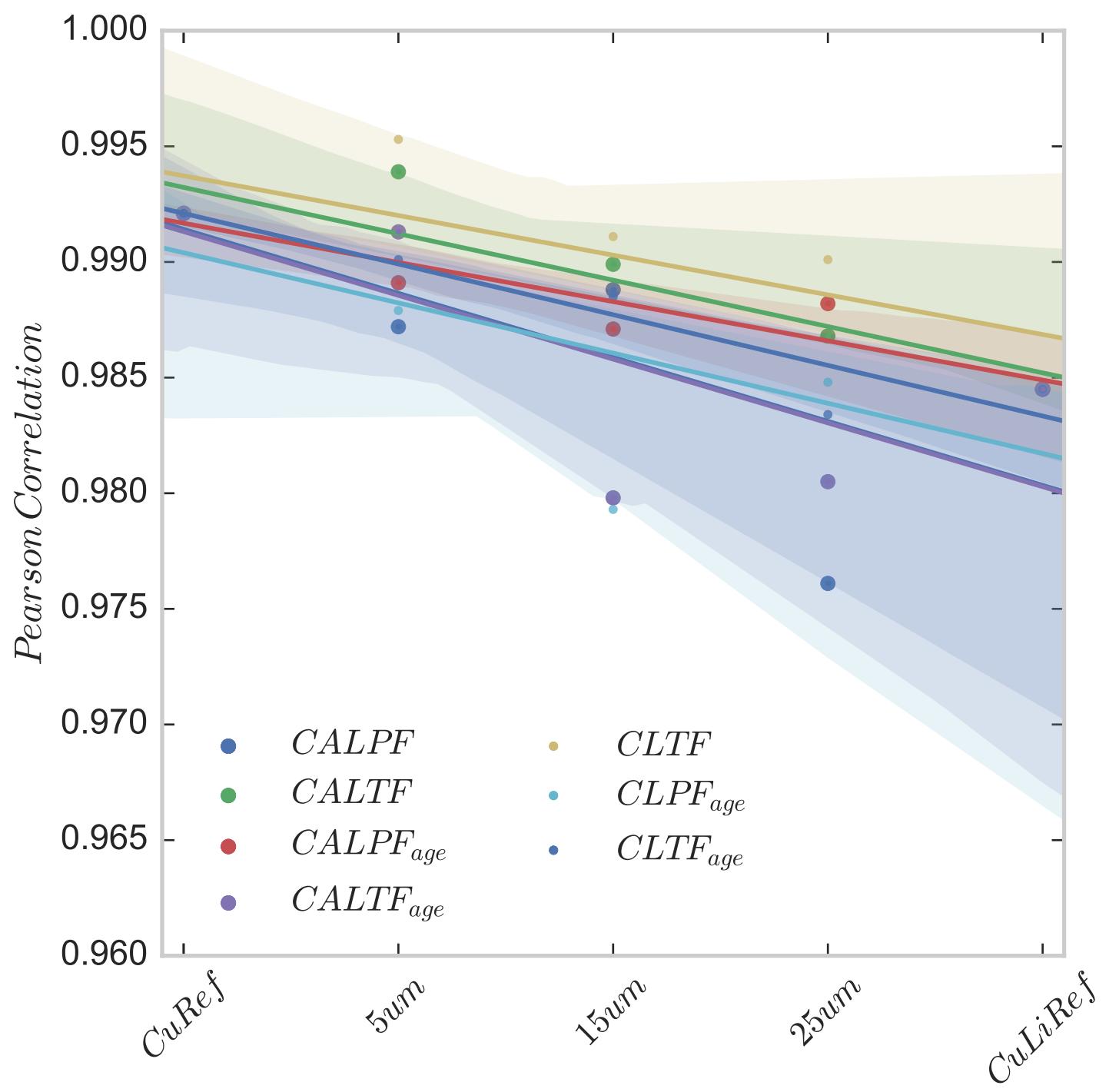


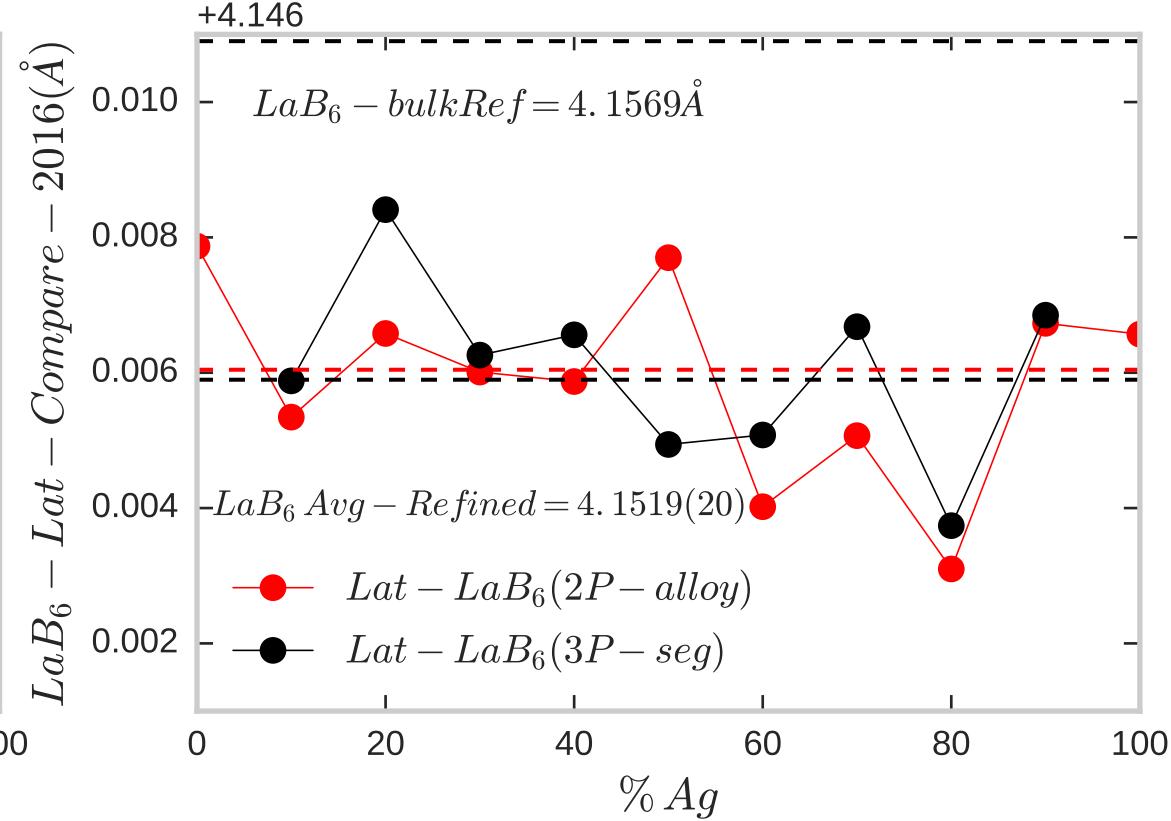
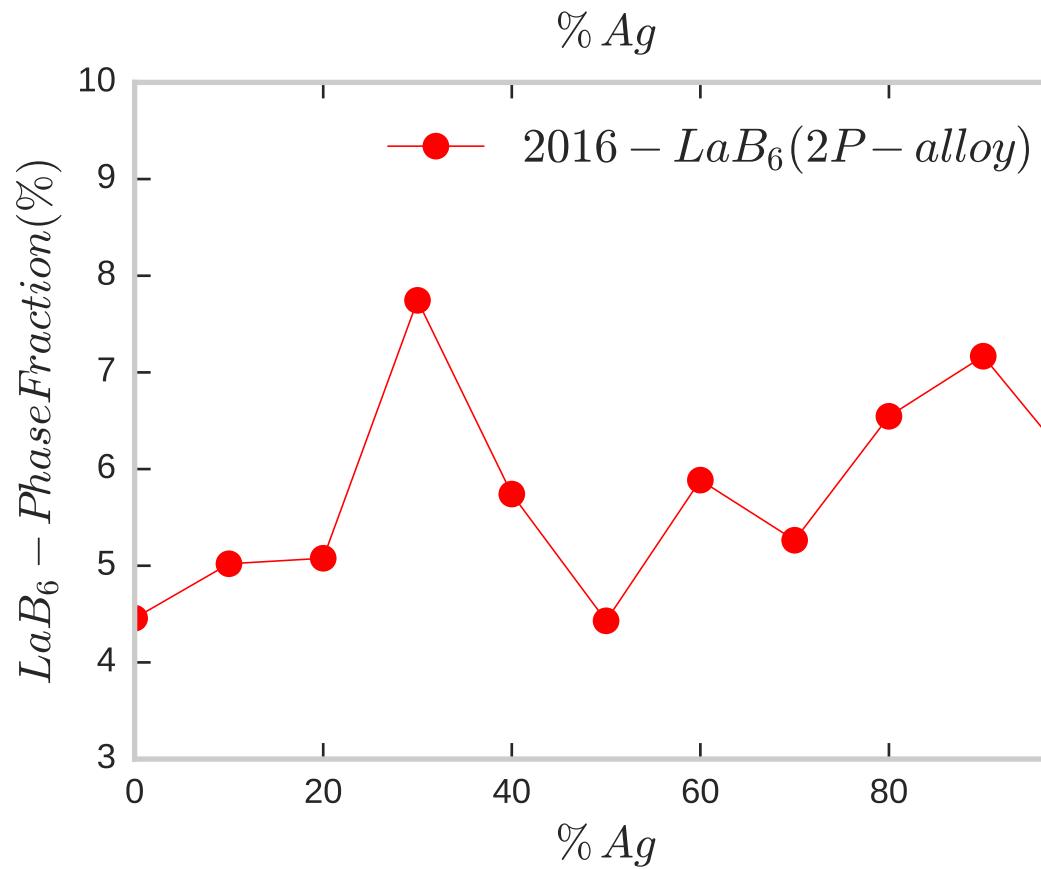
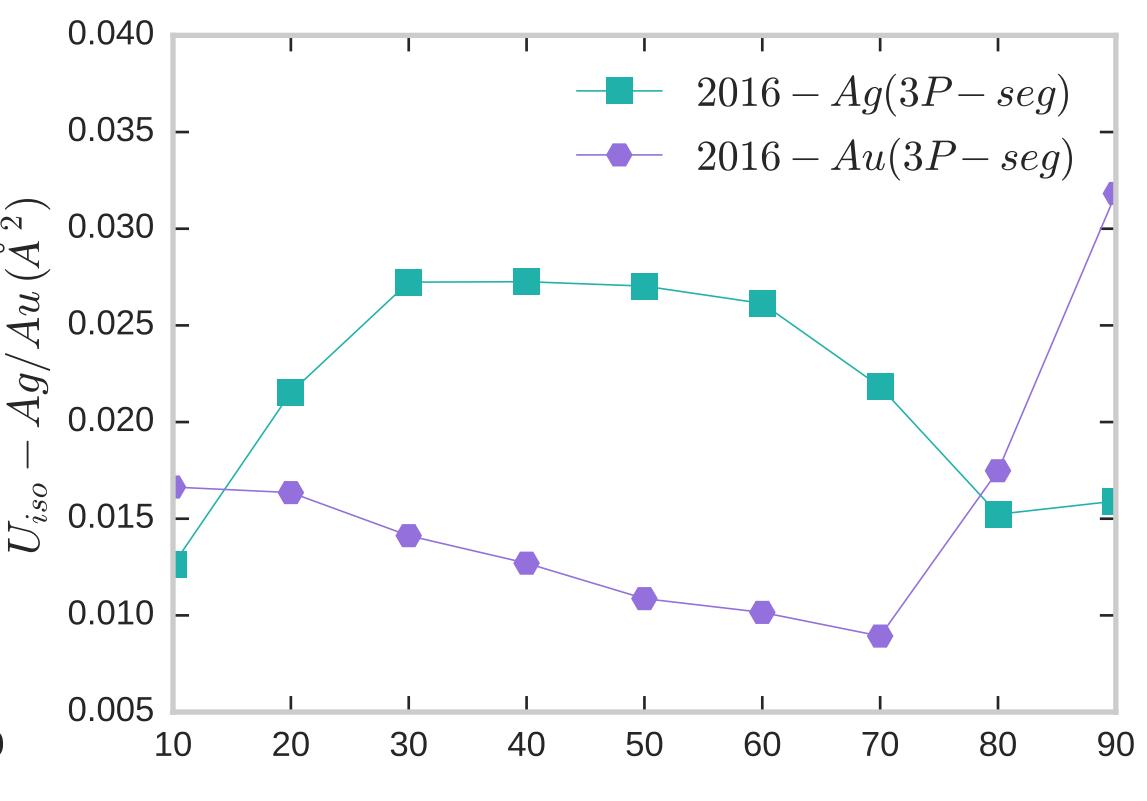
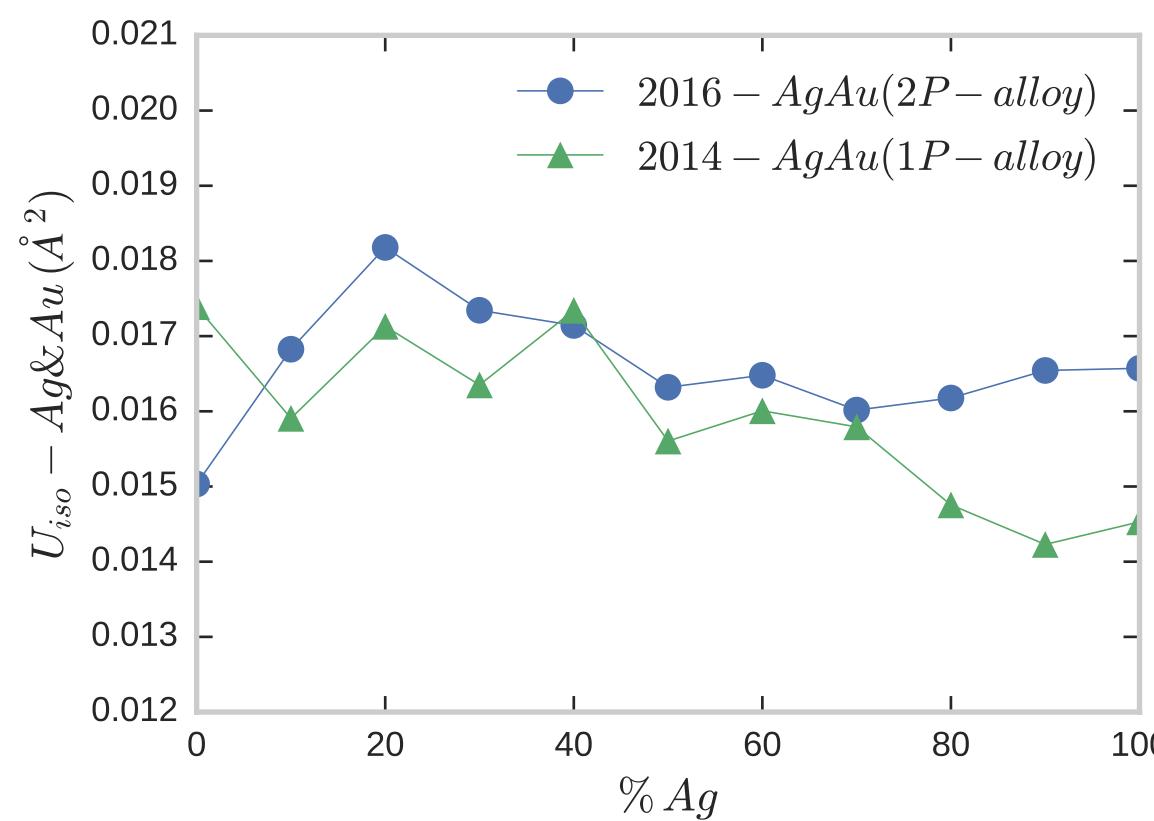
*Ag*

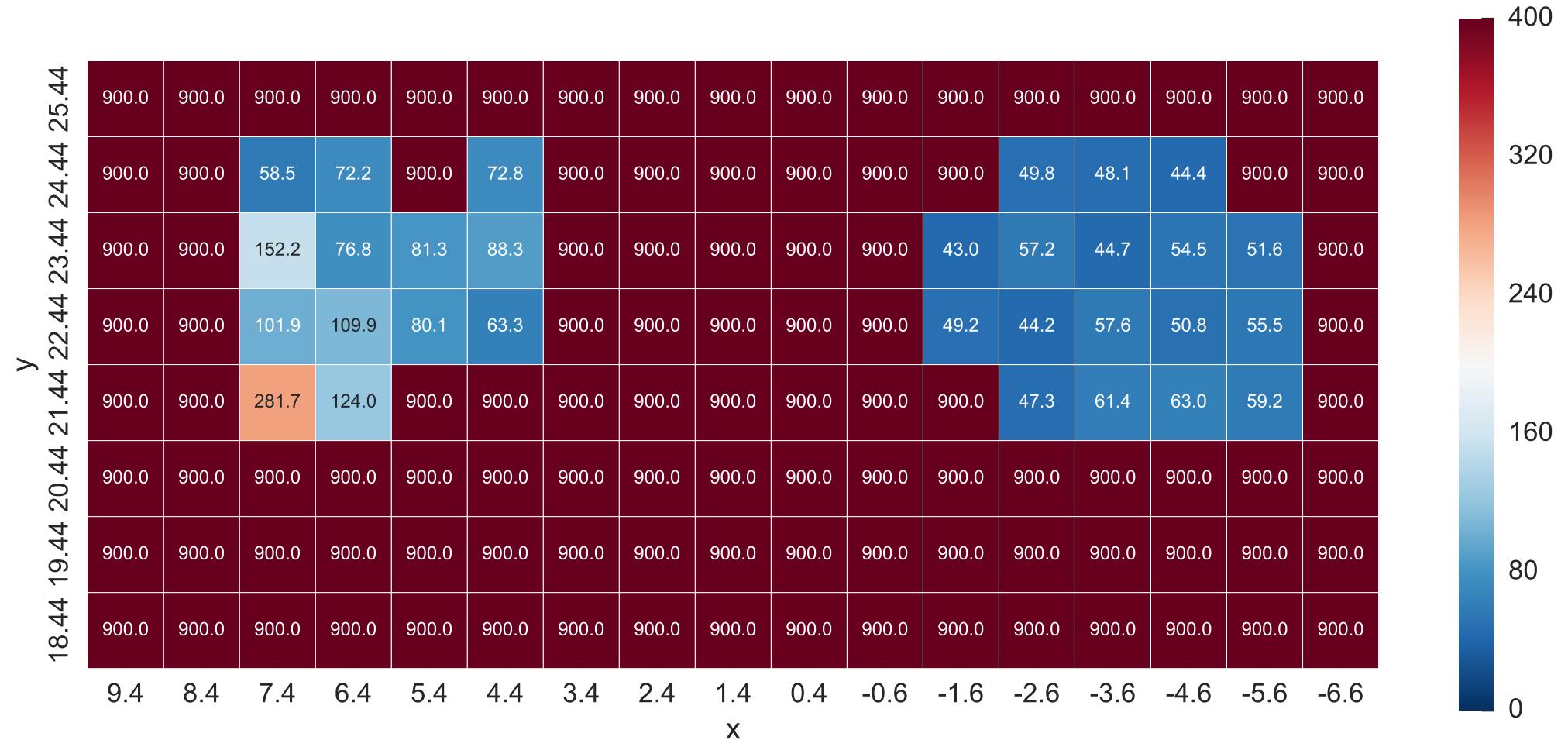


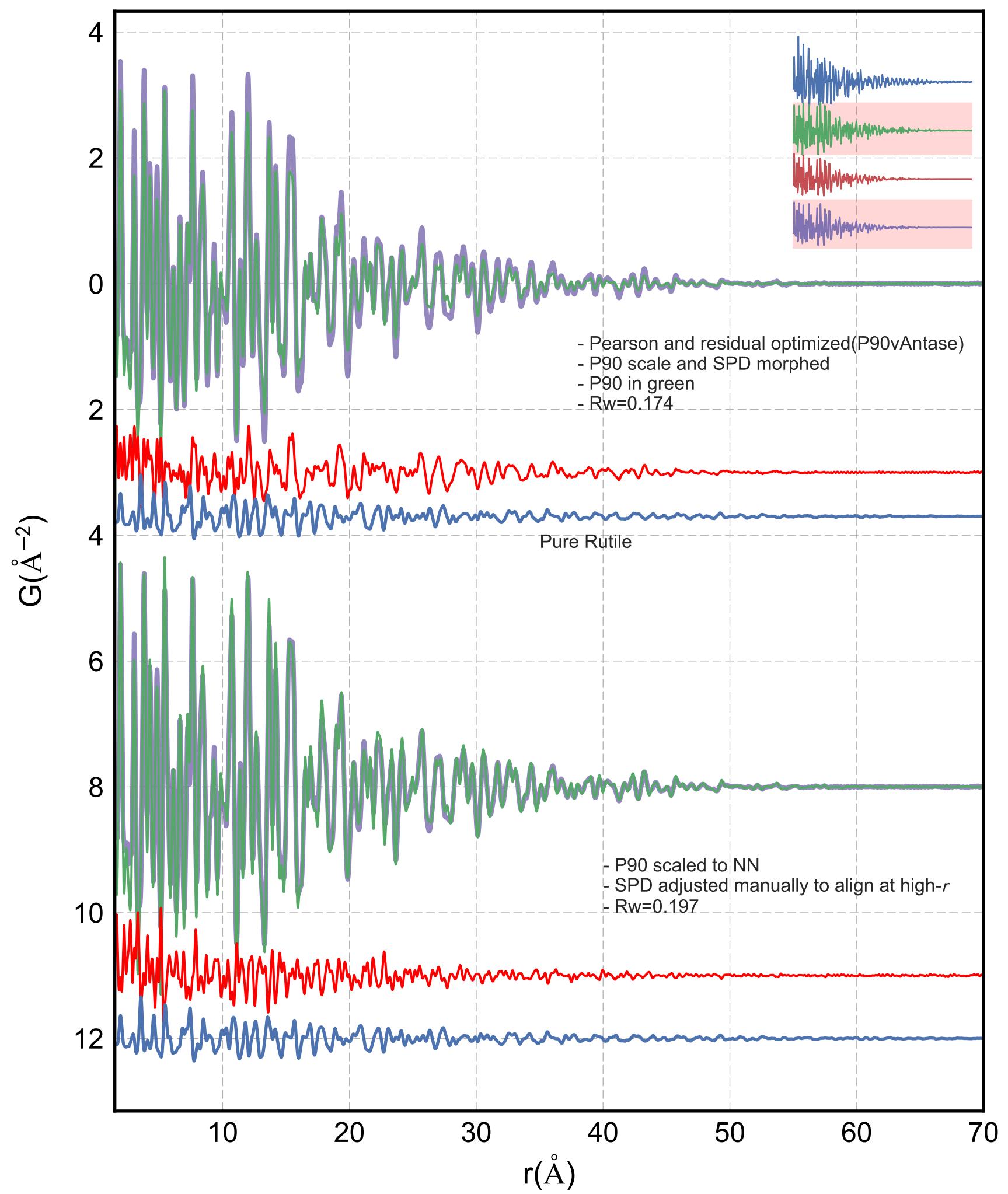


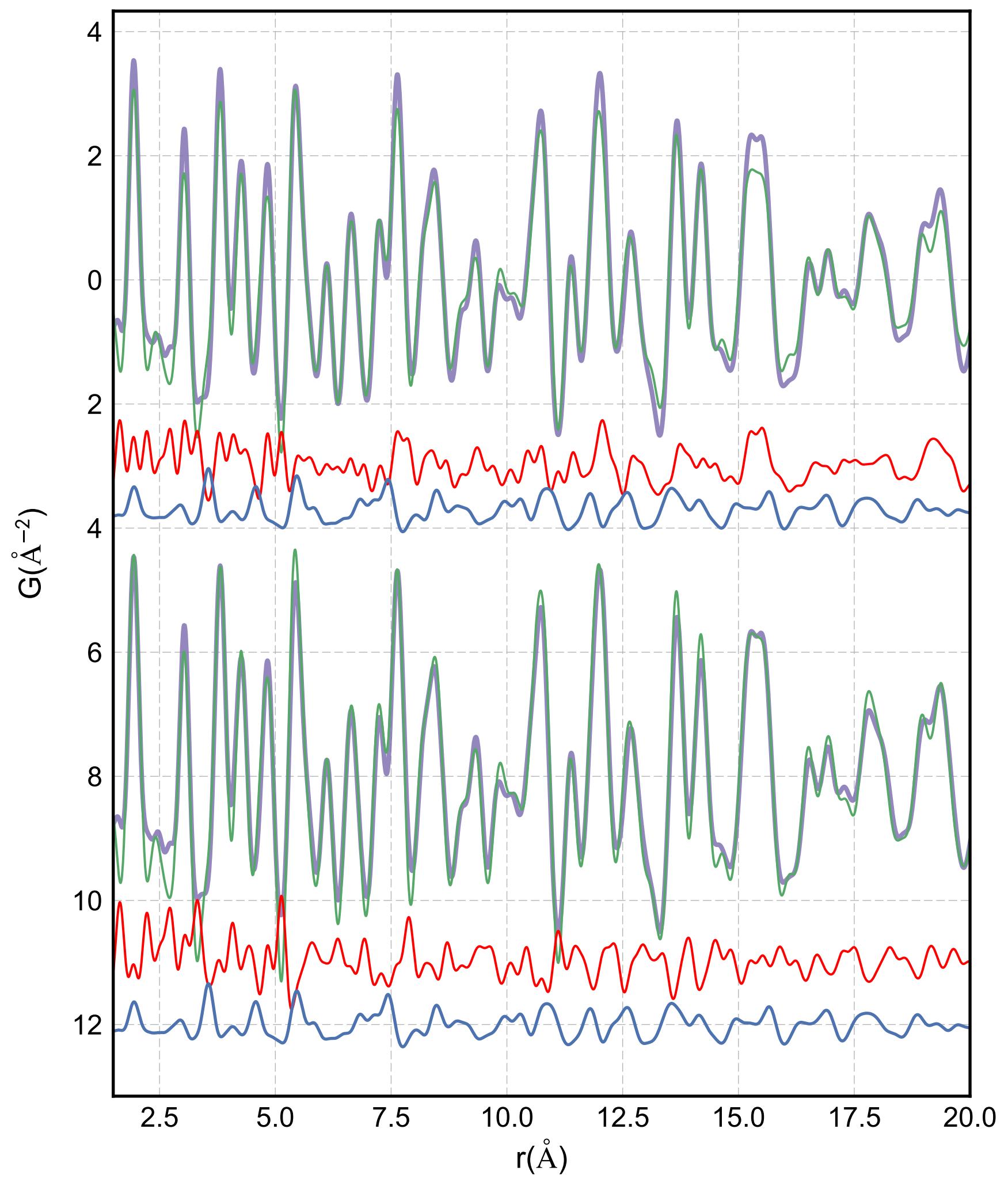


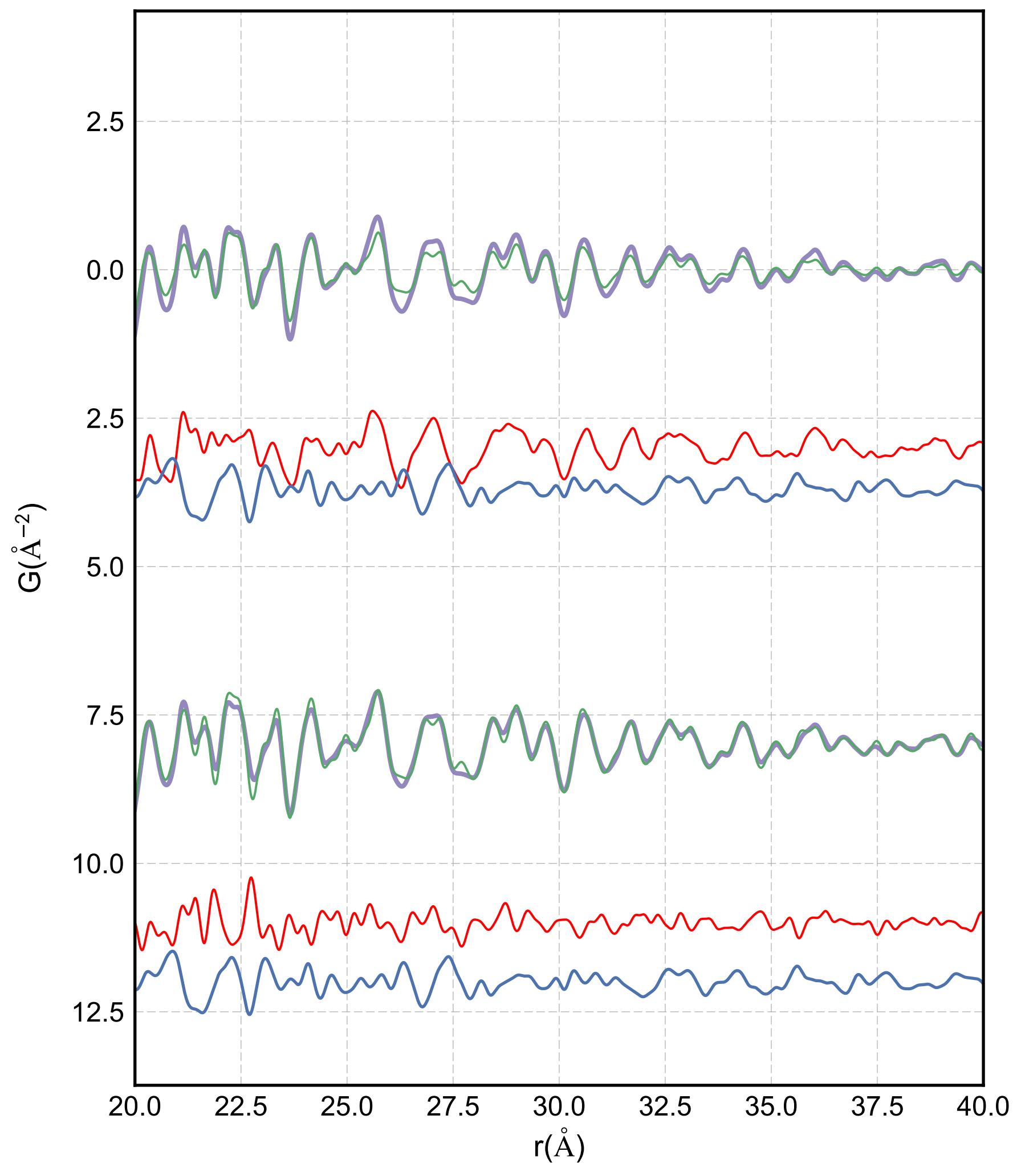


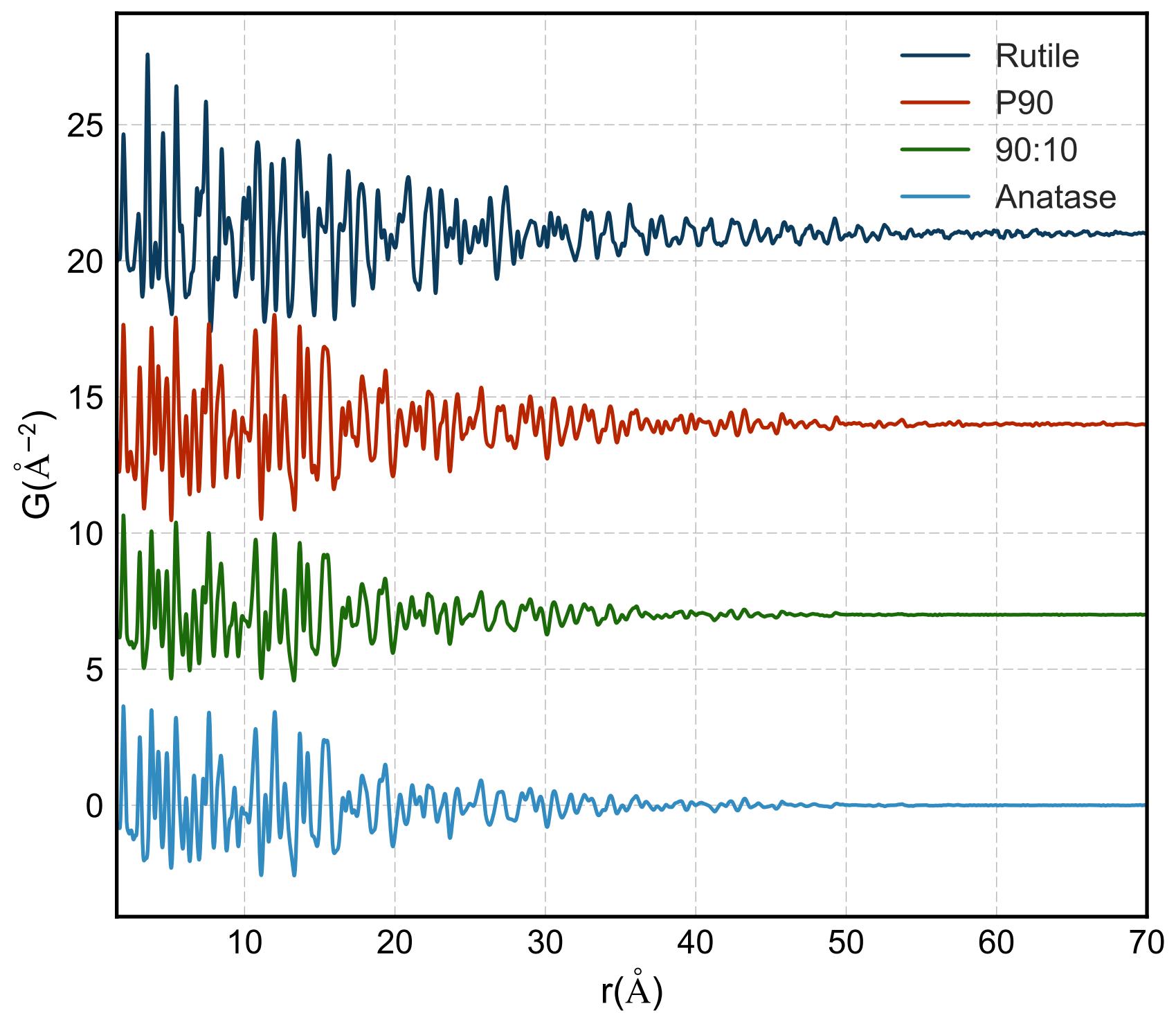


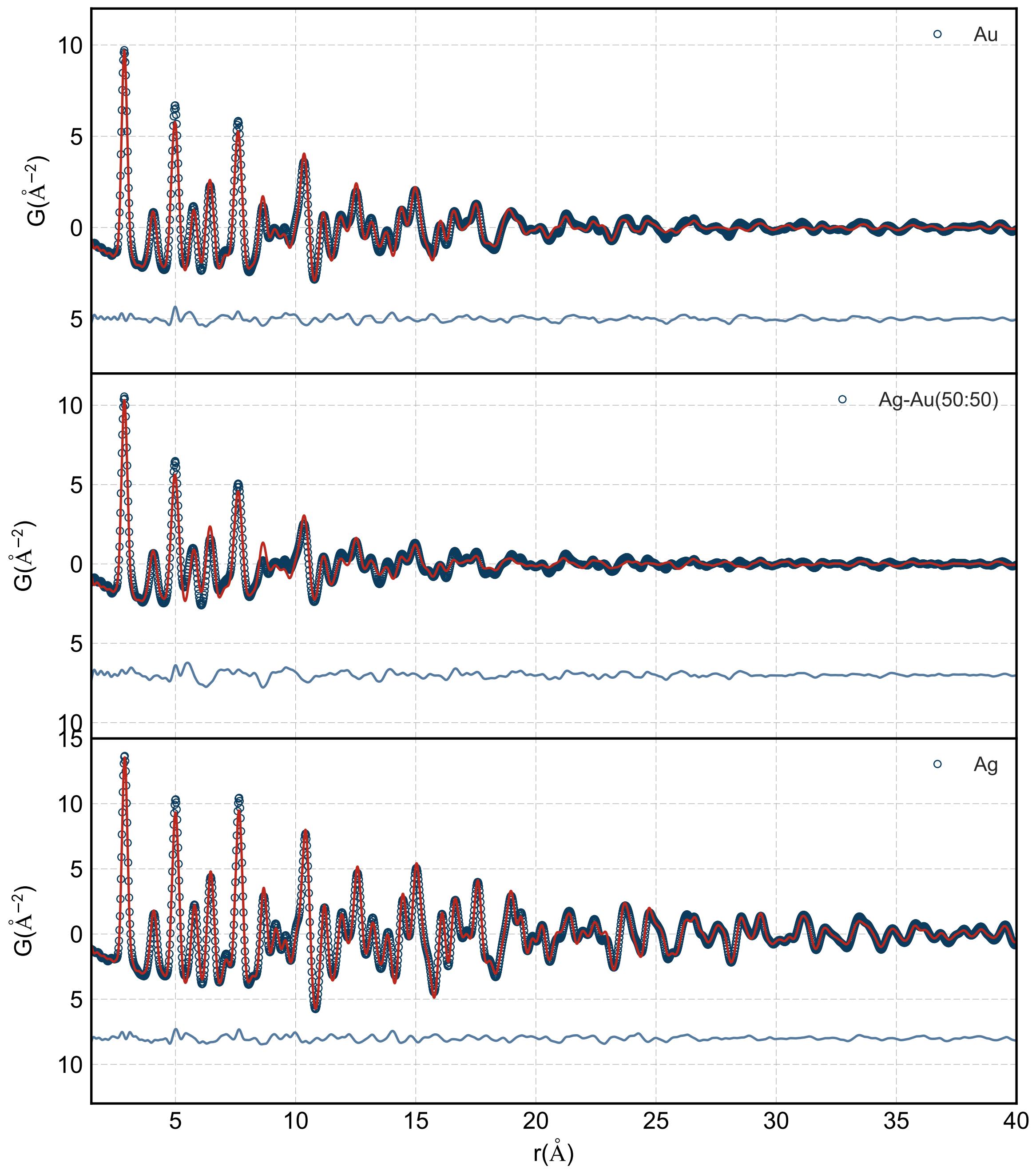


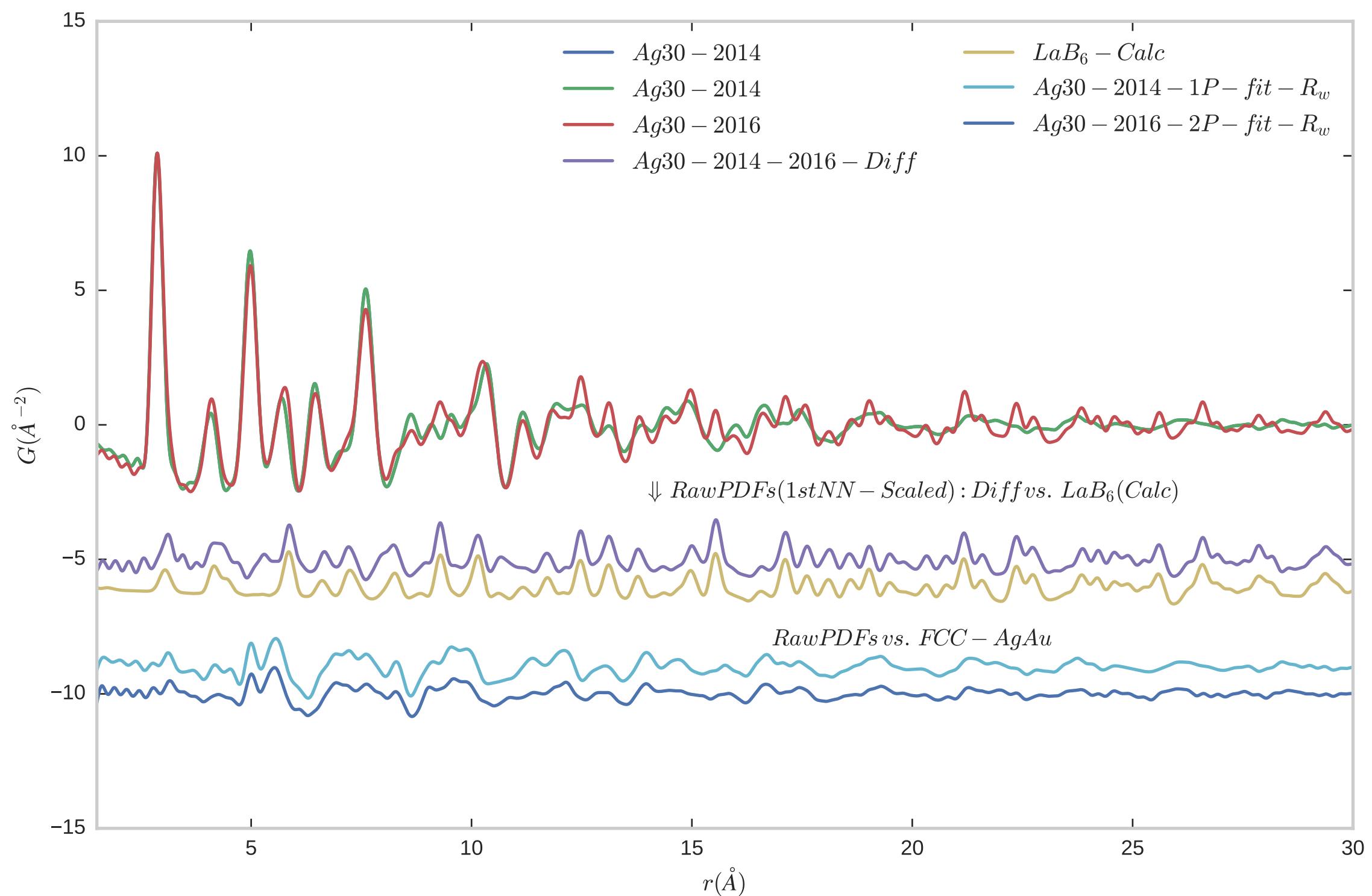






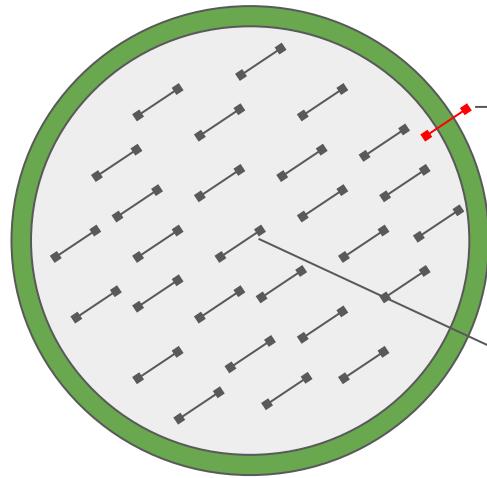








CS-Model (low-R)



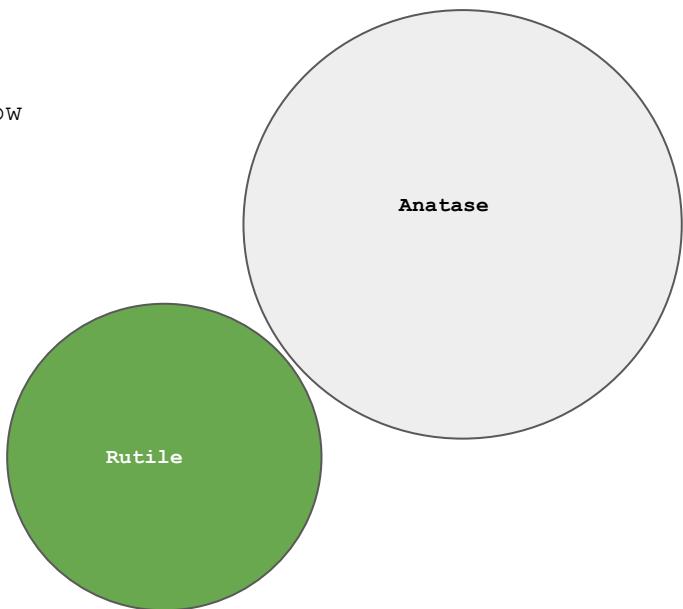
P-size: >25nm

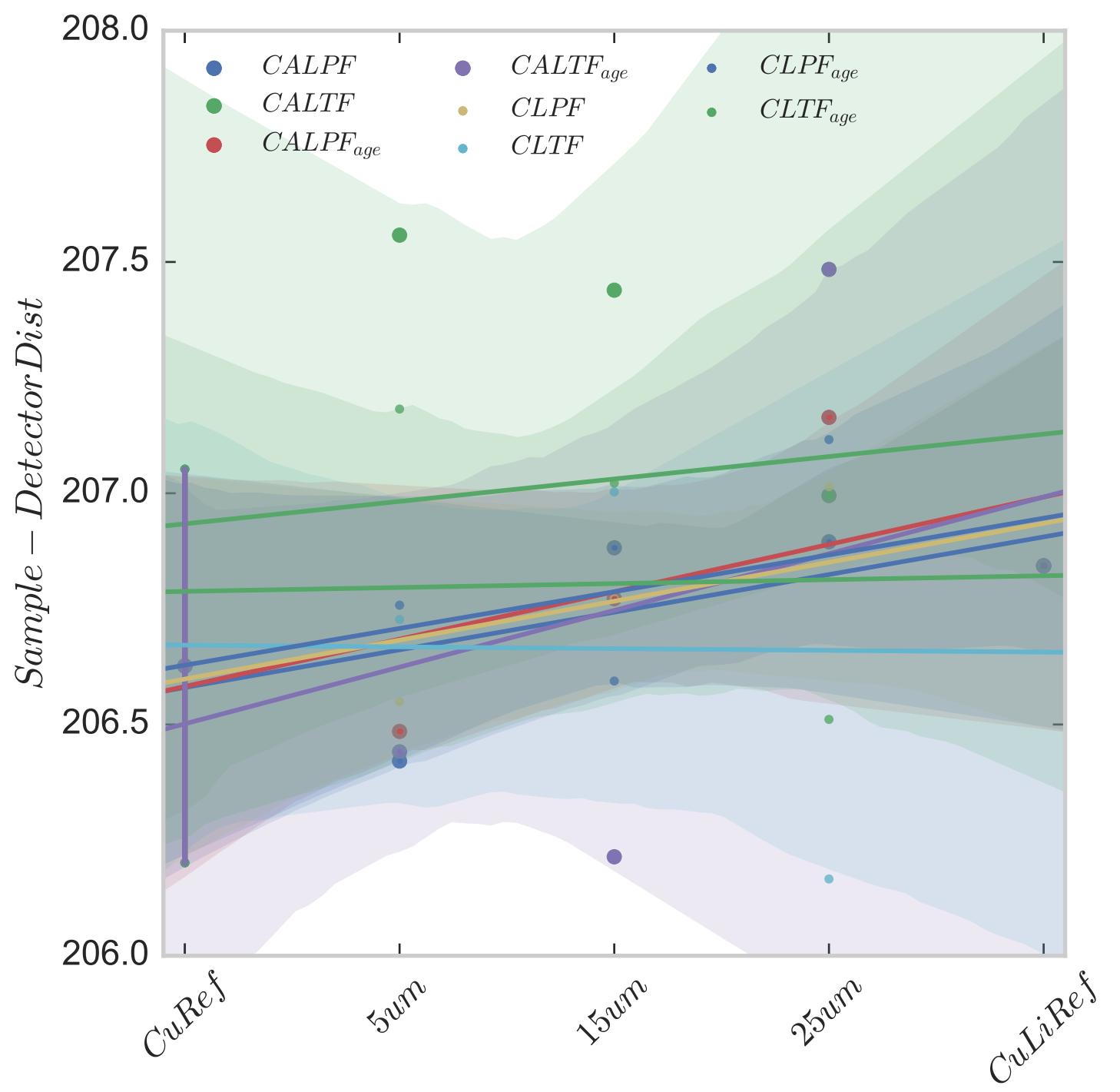
WAXS resolution: ~7-8nm

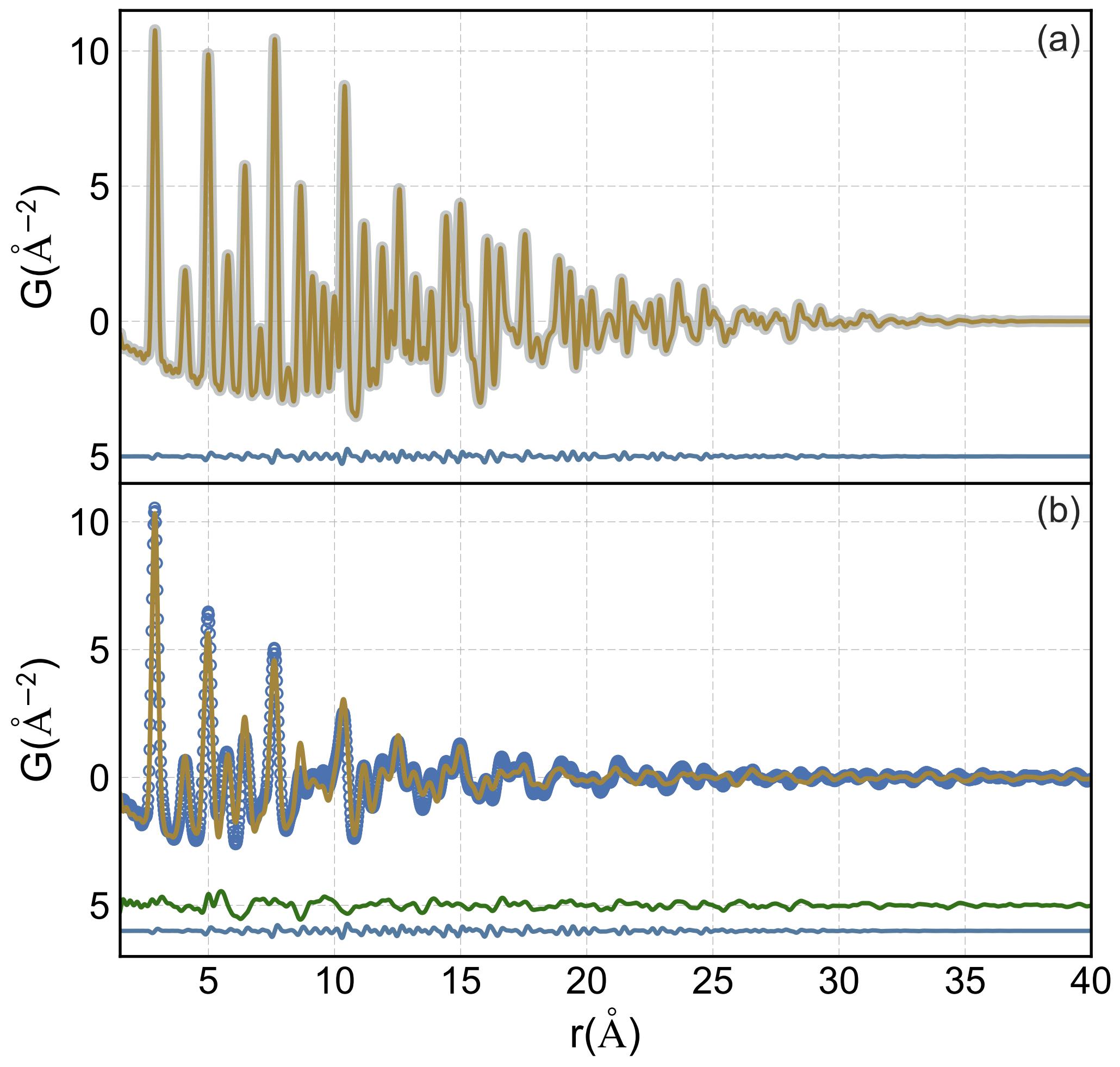
Rutile Correlations (low-R, low probability/phase %, reduced coherence)

Anatase Correlations (low-R, high probability/phase %, LRO coherence)

Poly-Model







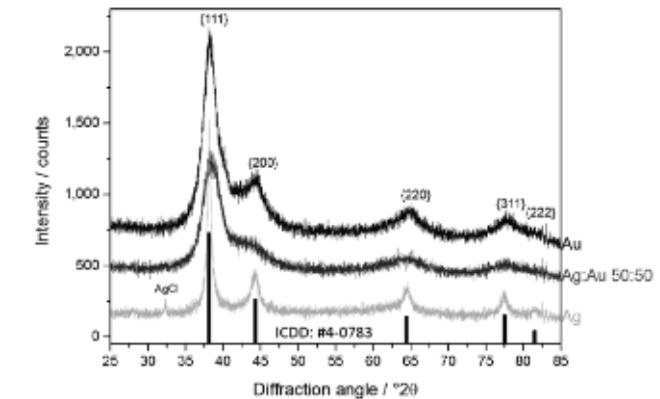
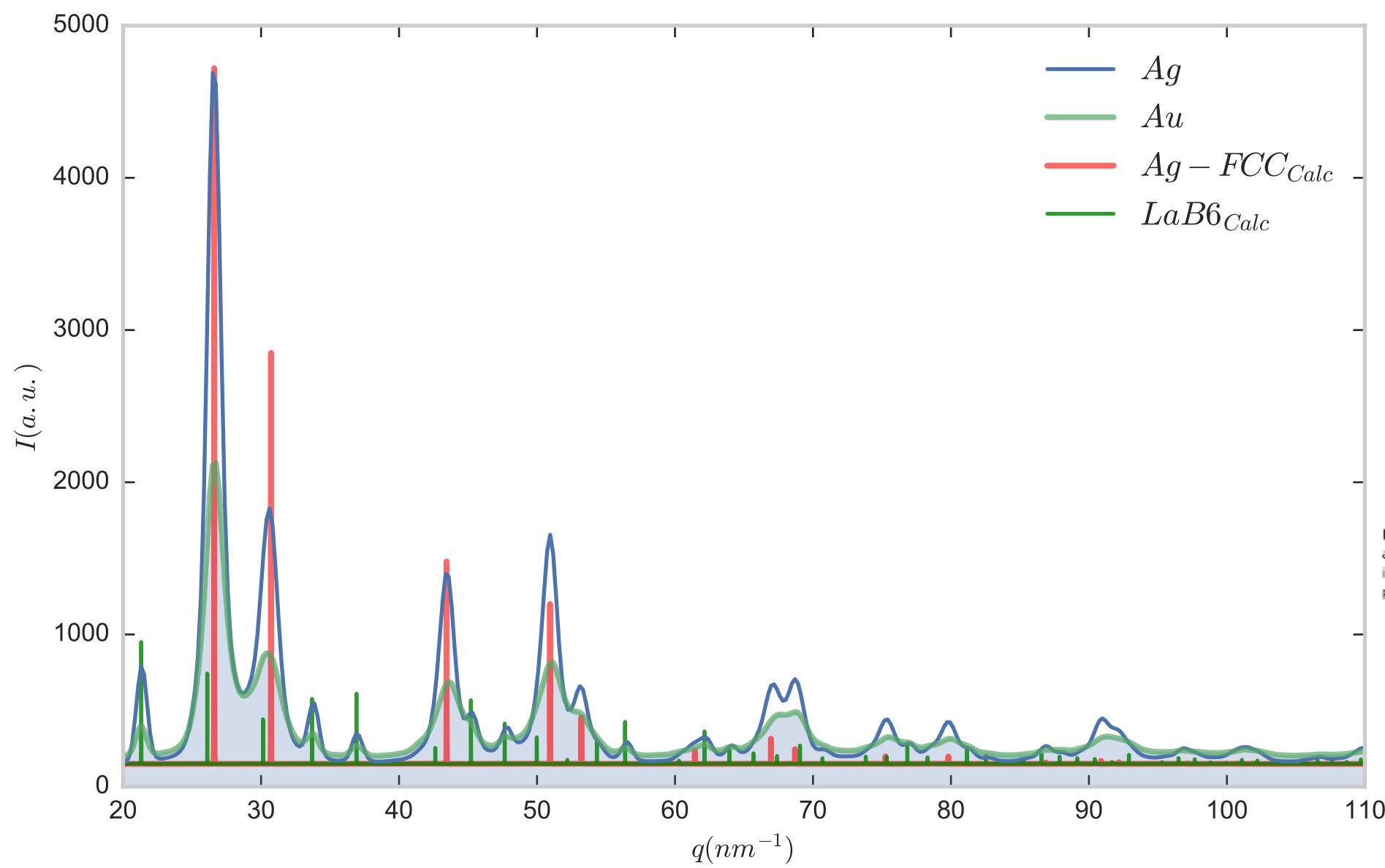


Fig. 5 Representative X-ray powder diffractograms of  $\text{Au}$ ,  $\text{Ag} : \text{Au} 50 : 50$ , and  $\text{Ag}$  nanoparticles. At the bottom, the peaks of elemental silver are indicated. Note the traces of  $\text{AgCl}$  from the synthesis which were found in pure silver nanoparticles.

