

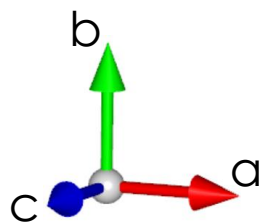
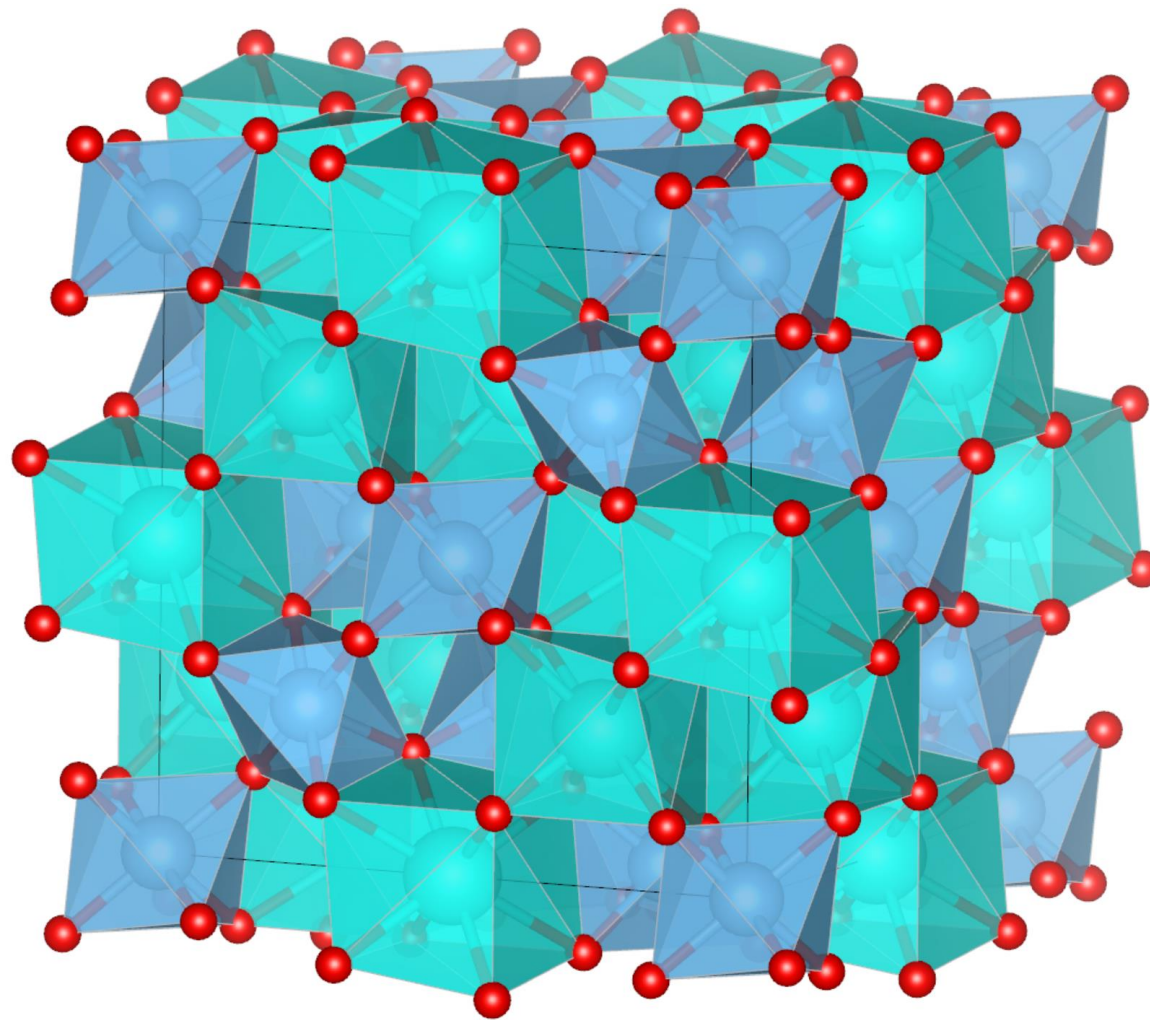
Summary of RMC modeling for $\text{Yb}_2\text{Ti}_{2-2x}\text{Sn}_{2x}\text{O}_7$ neutron total scattering data

Yuanpeng Zhang

Neutron Scattering Division

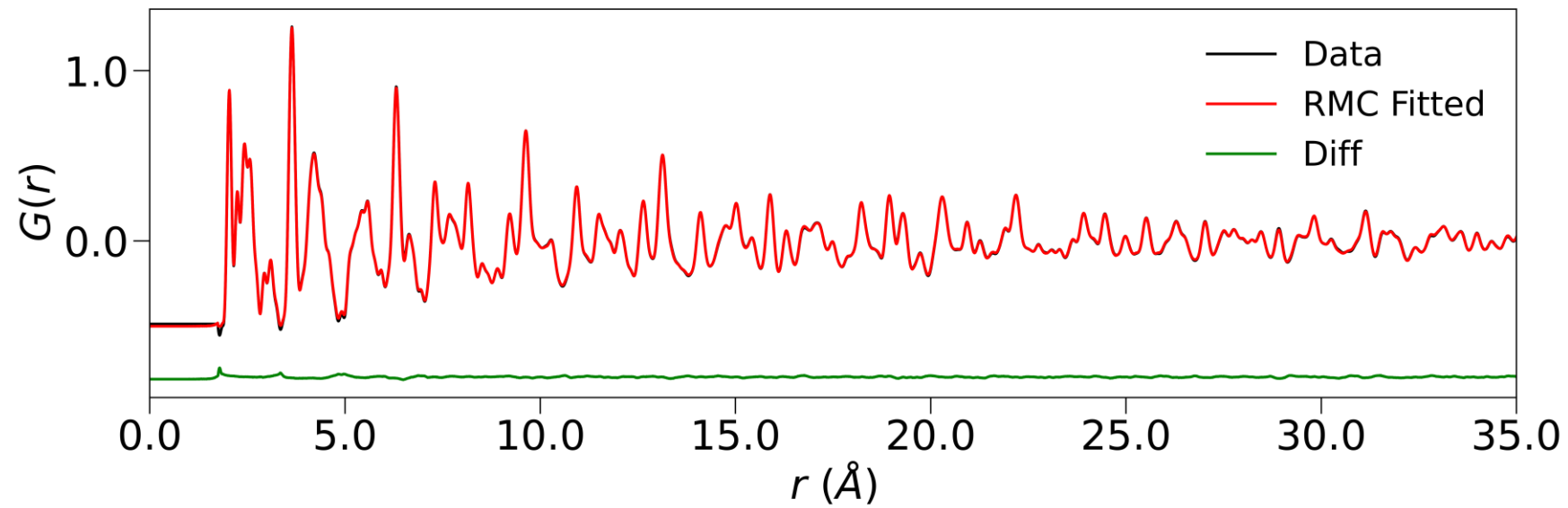
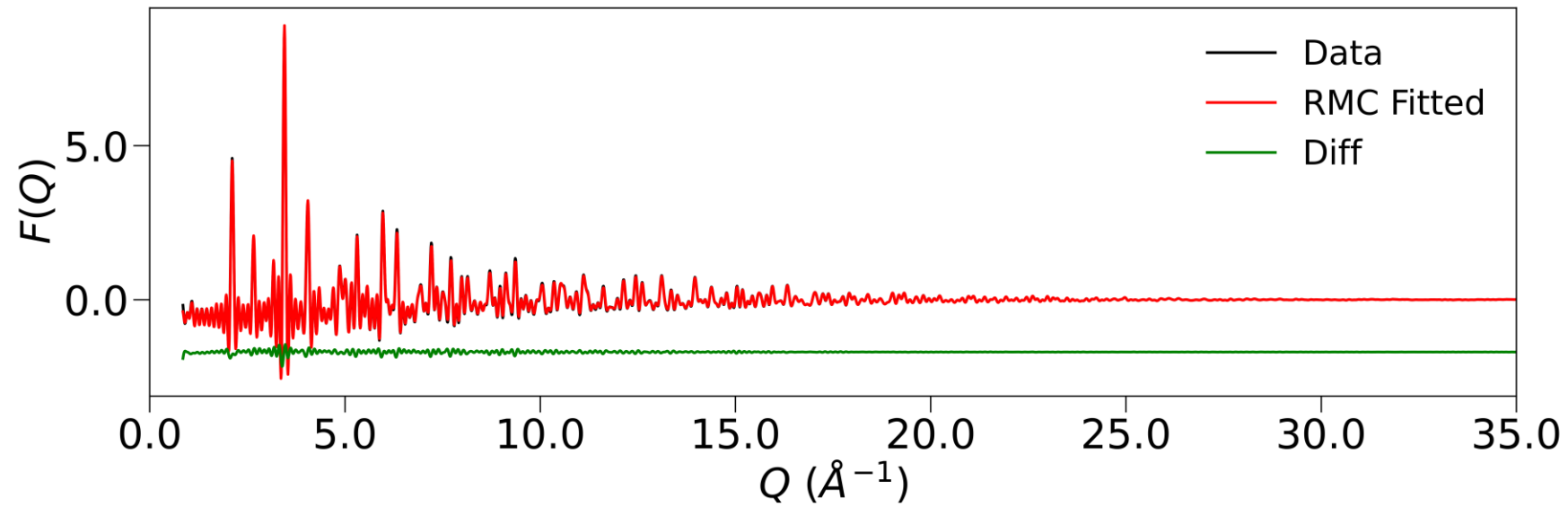
Dec-14-2022

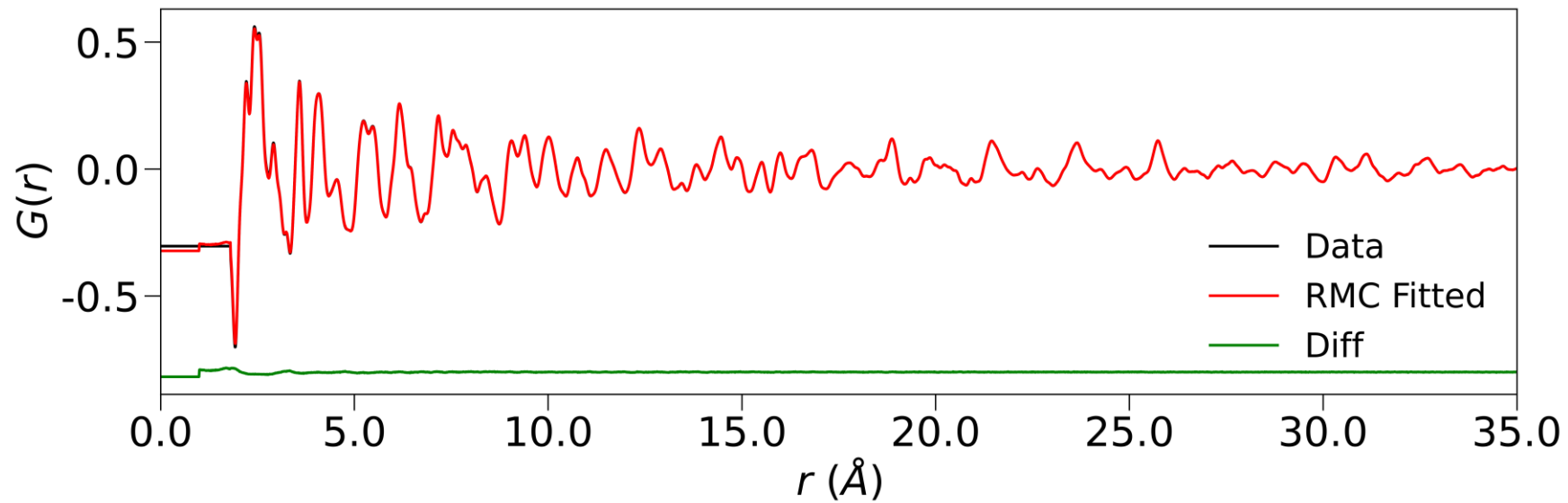
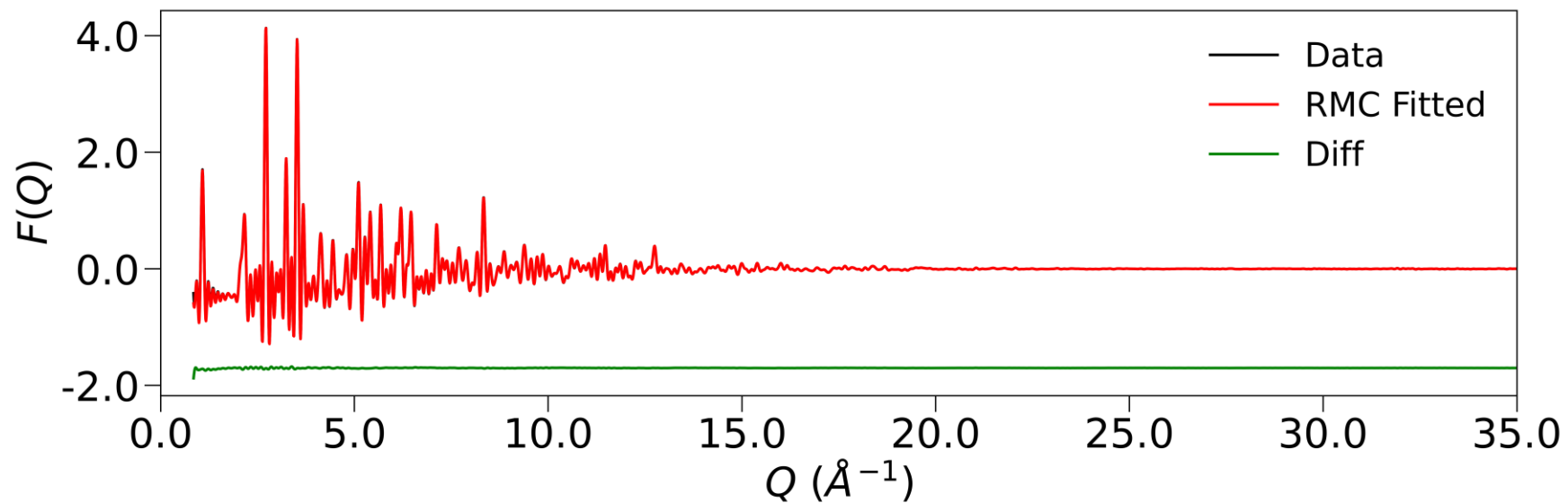
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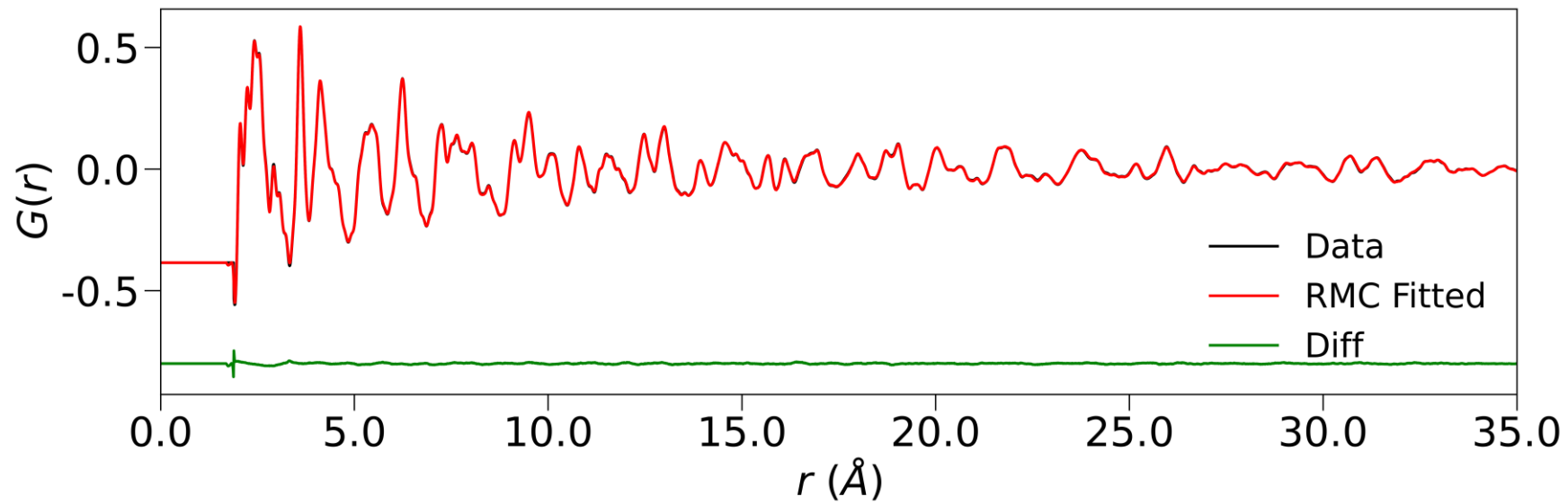
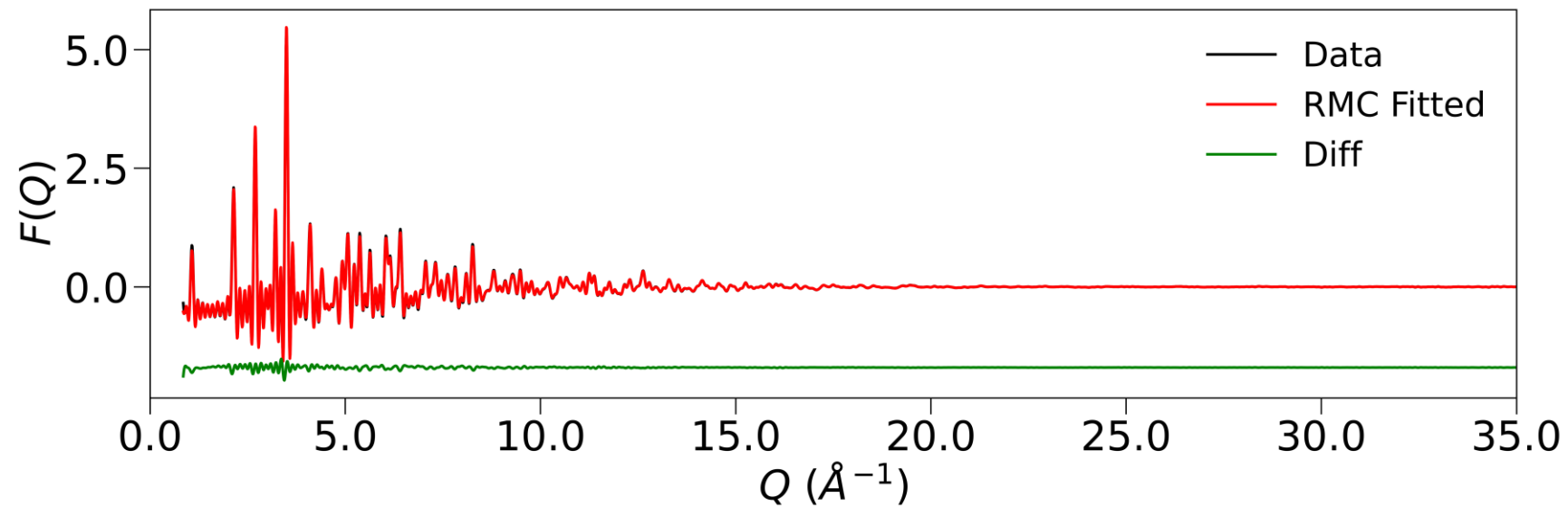


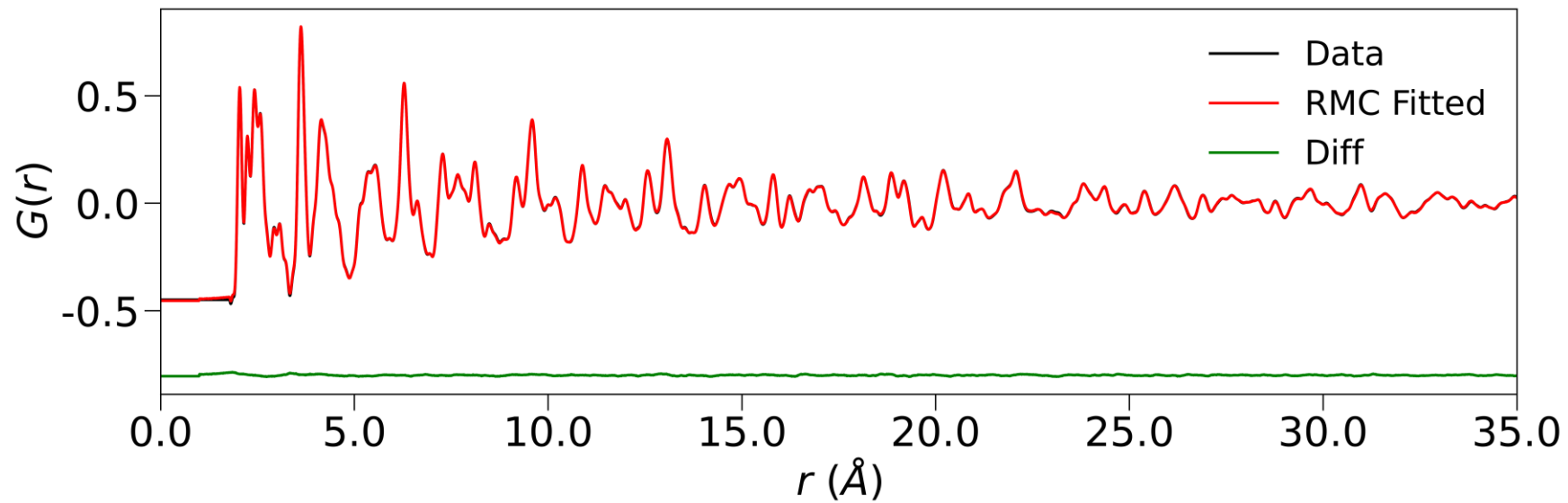
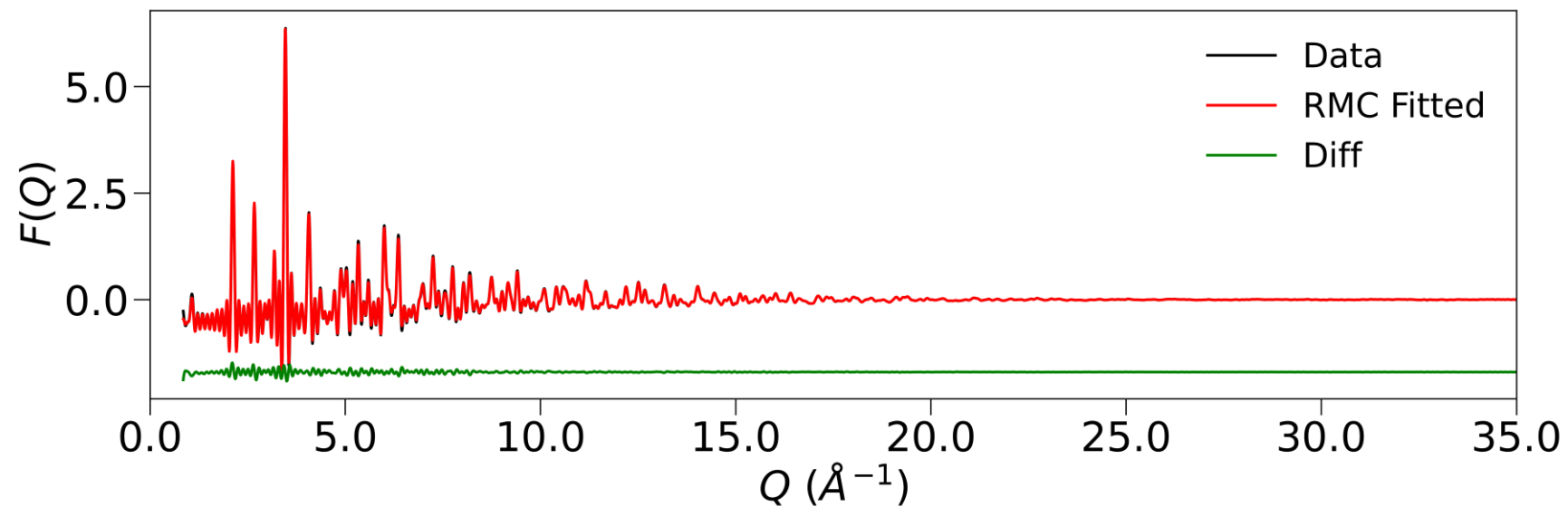
- ❖ Unit cell expanded to 10x10x10 supercell and symmetry constraint removed.
- ❖ Modeling were driven purely by experimental data.
- ❖ Conventional metropolis Monte Carlo routine used.
- ❖ Bragg data not included due to the complexity with average structure. Thus, we only focus on the local scale correlation in real space.
- ❖ Both the reciprocal and real space data were included for the model refinement and the weight for each dataset was adjusted on-the-fly in an automatic manner.
- ❖ For doped sample, Ti atoms were replaced with Sn in the expanded supercell in a random manner according to the stoichiometry.
- ❖ On average, ~100 moves/atom were generated, among which ~20 moves/atom were accepted.

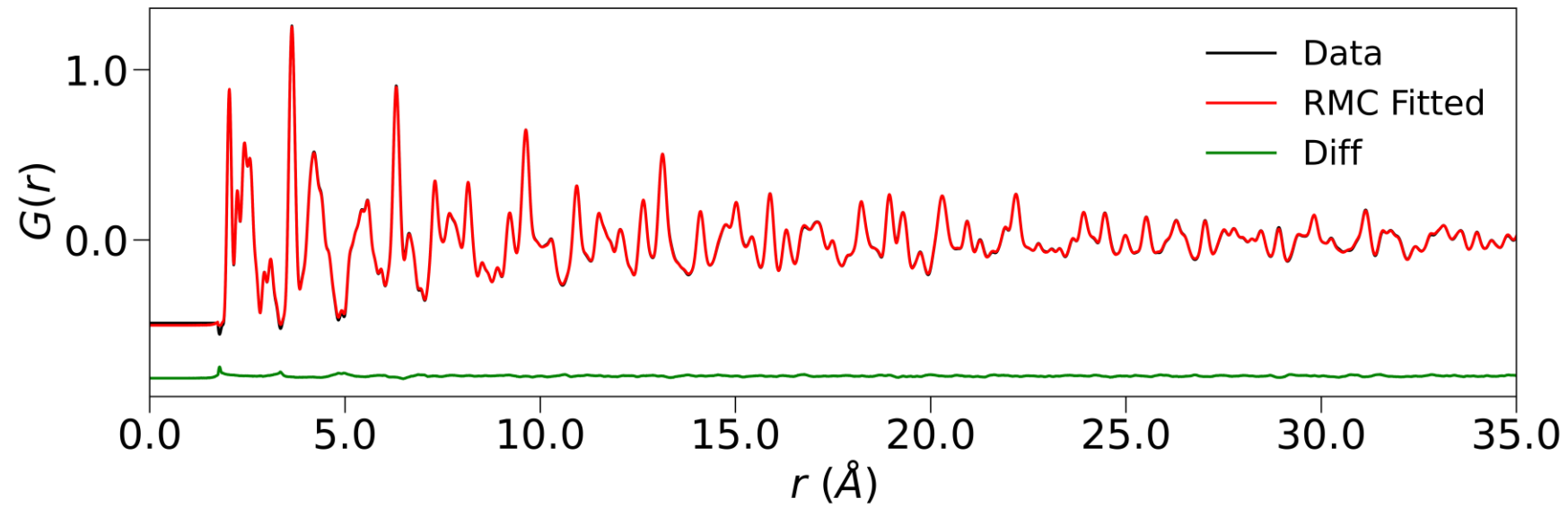
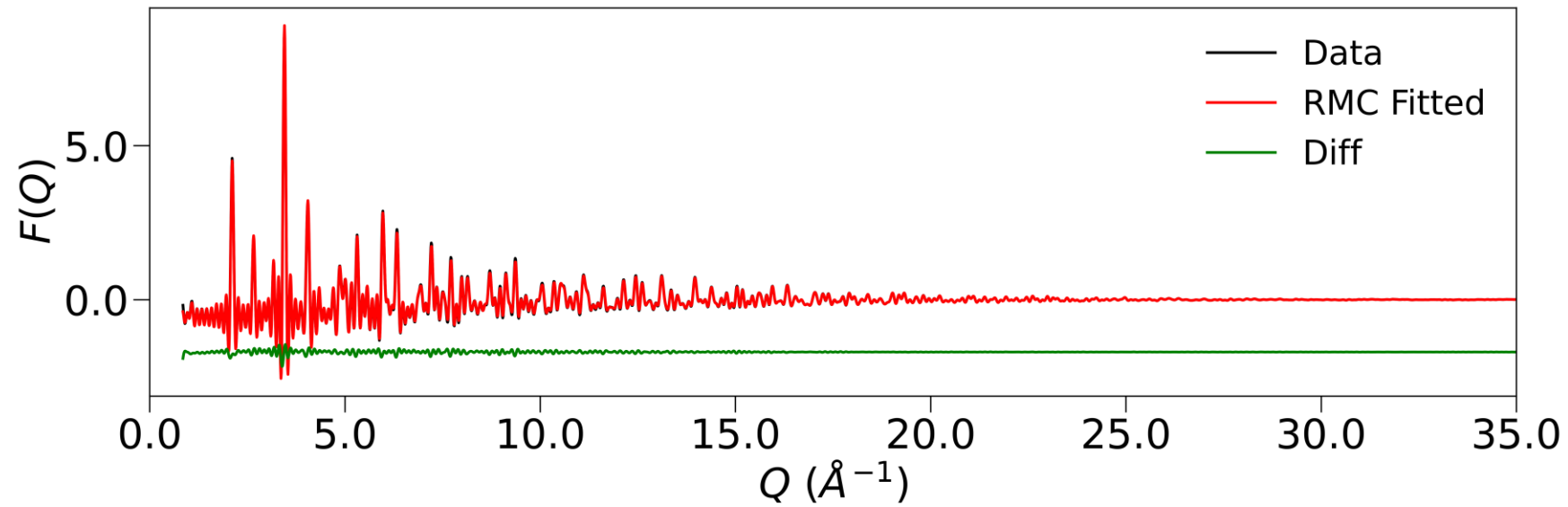
Total scattering data fitting





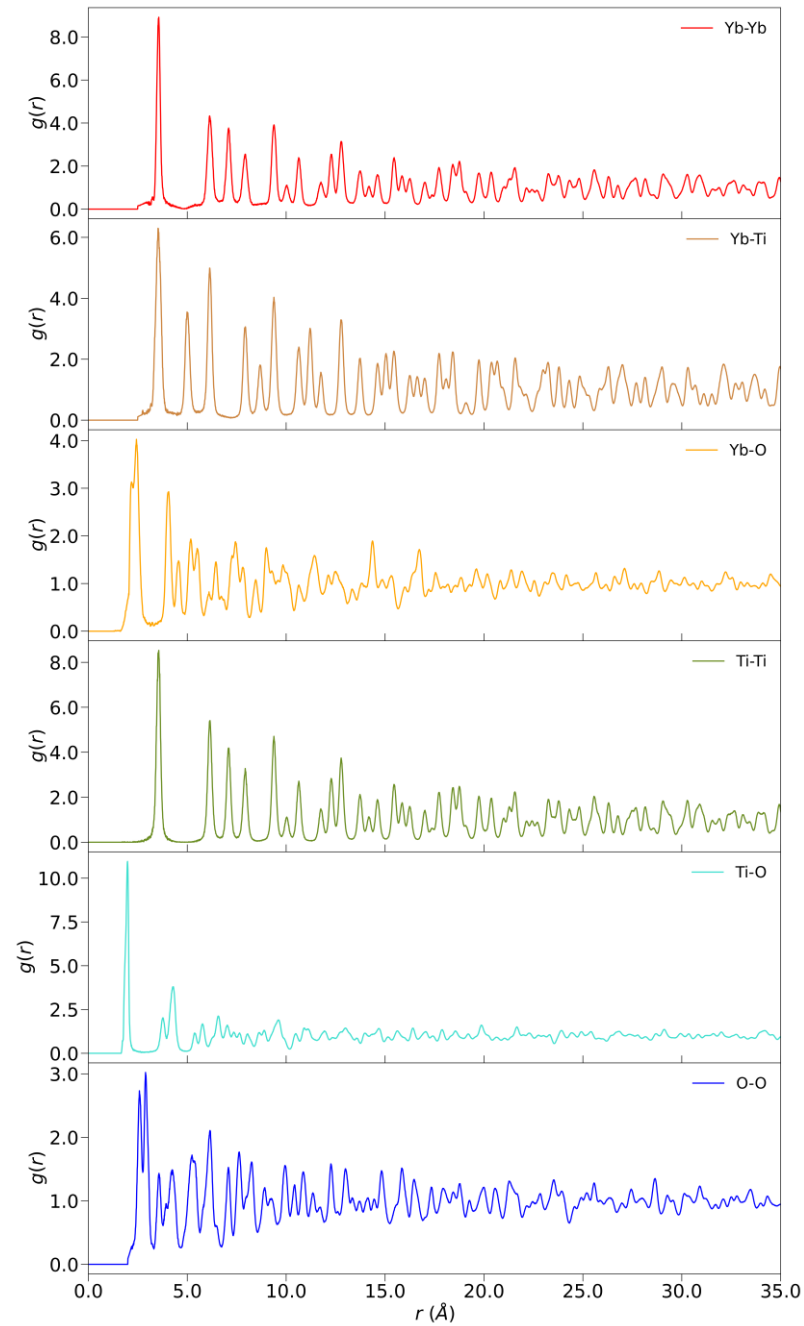


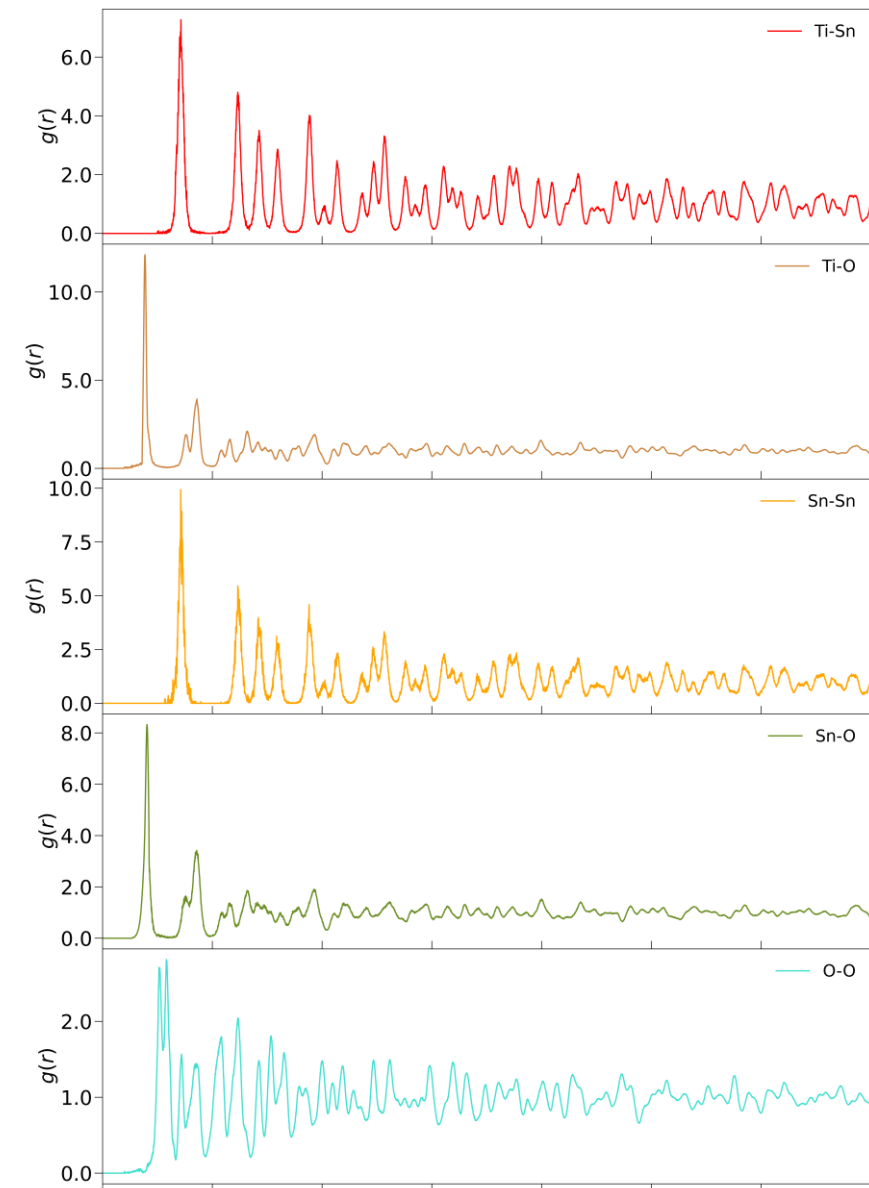
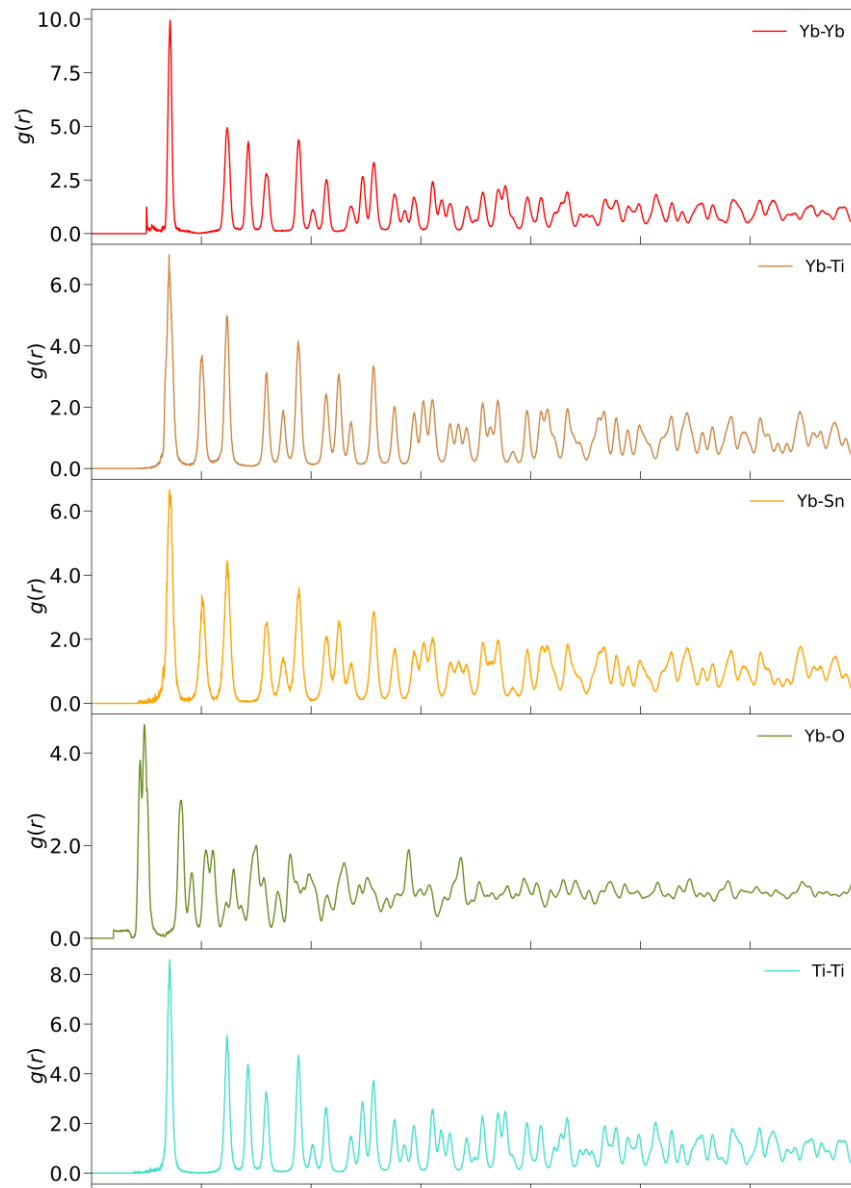


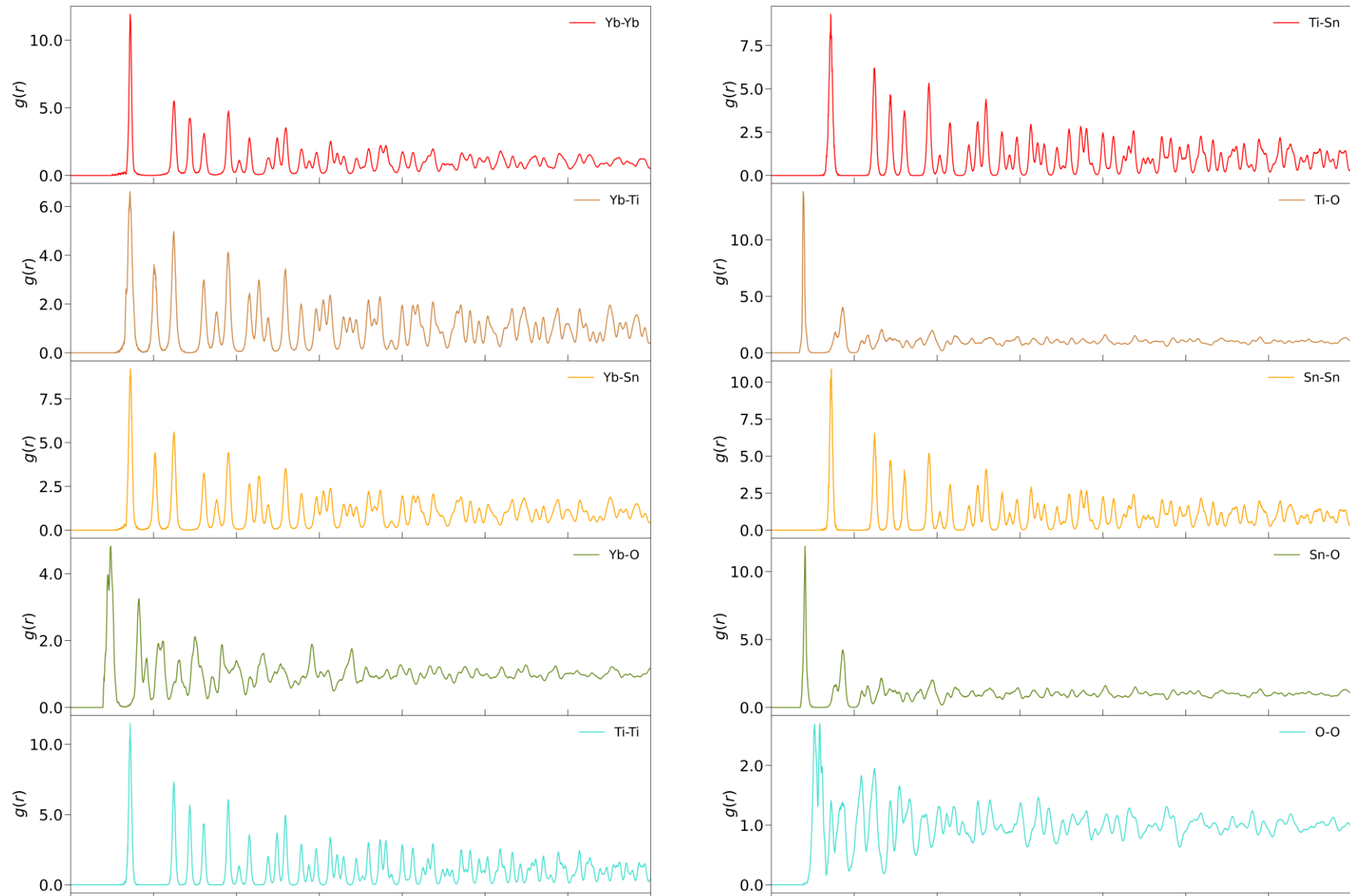


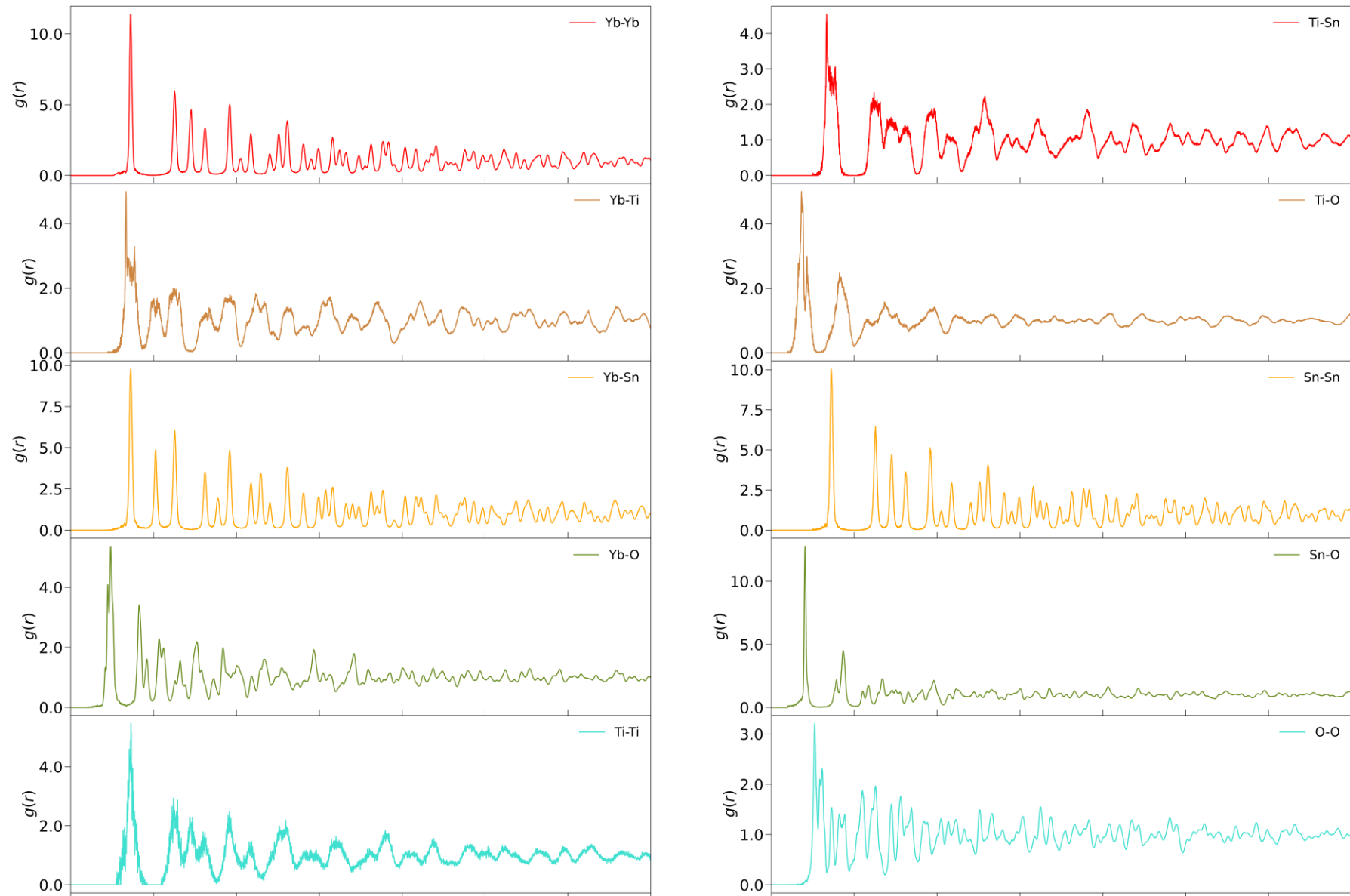
Overall, the fitting quality is reasonable in both spaces.

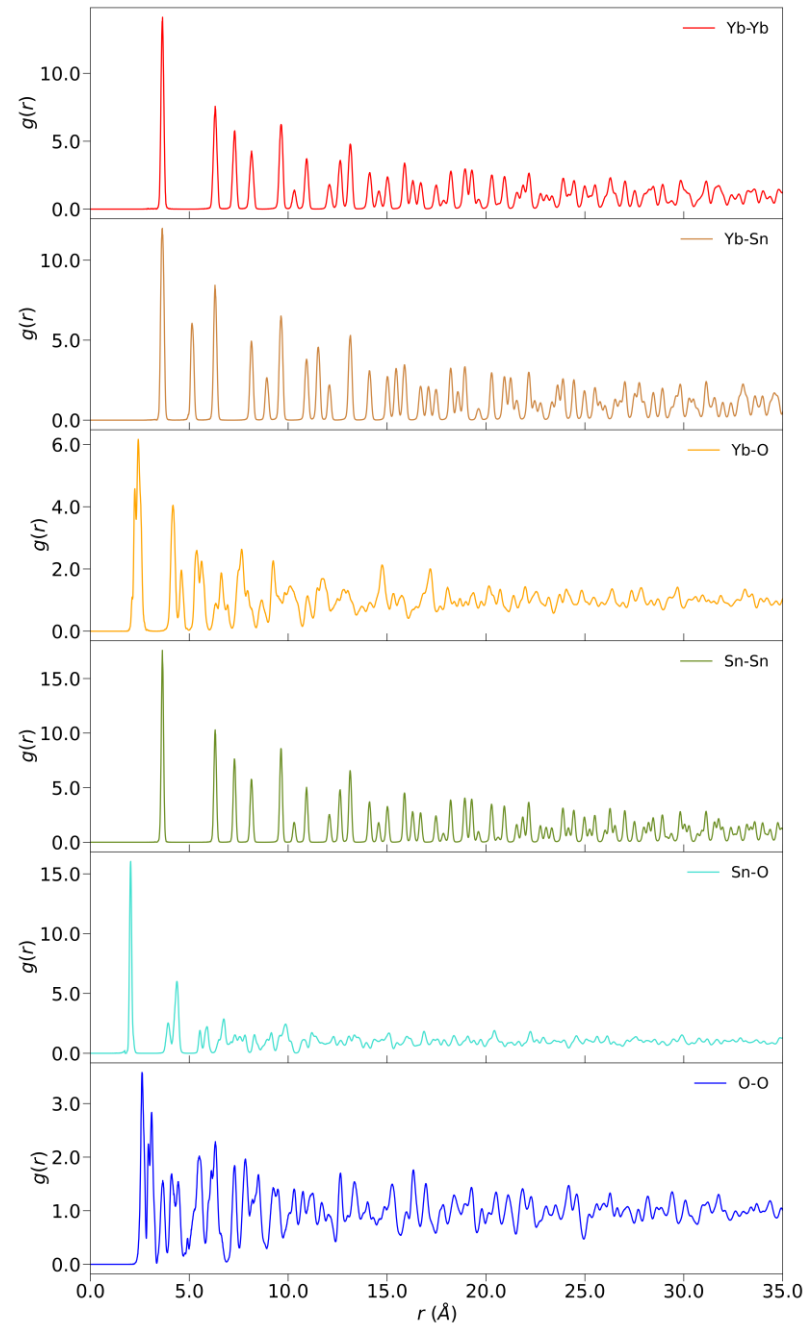
Partial PDFs



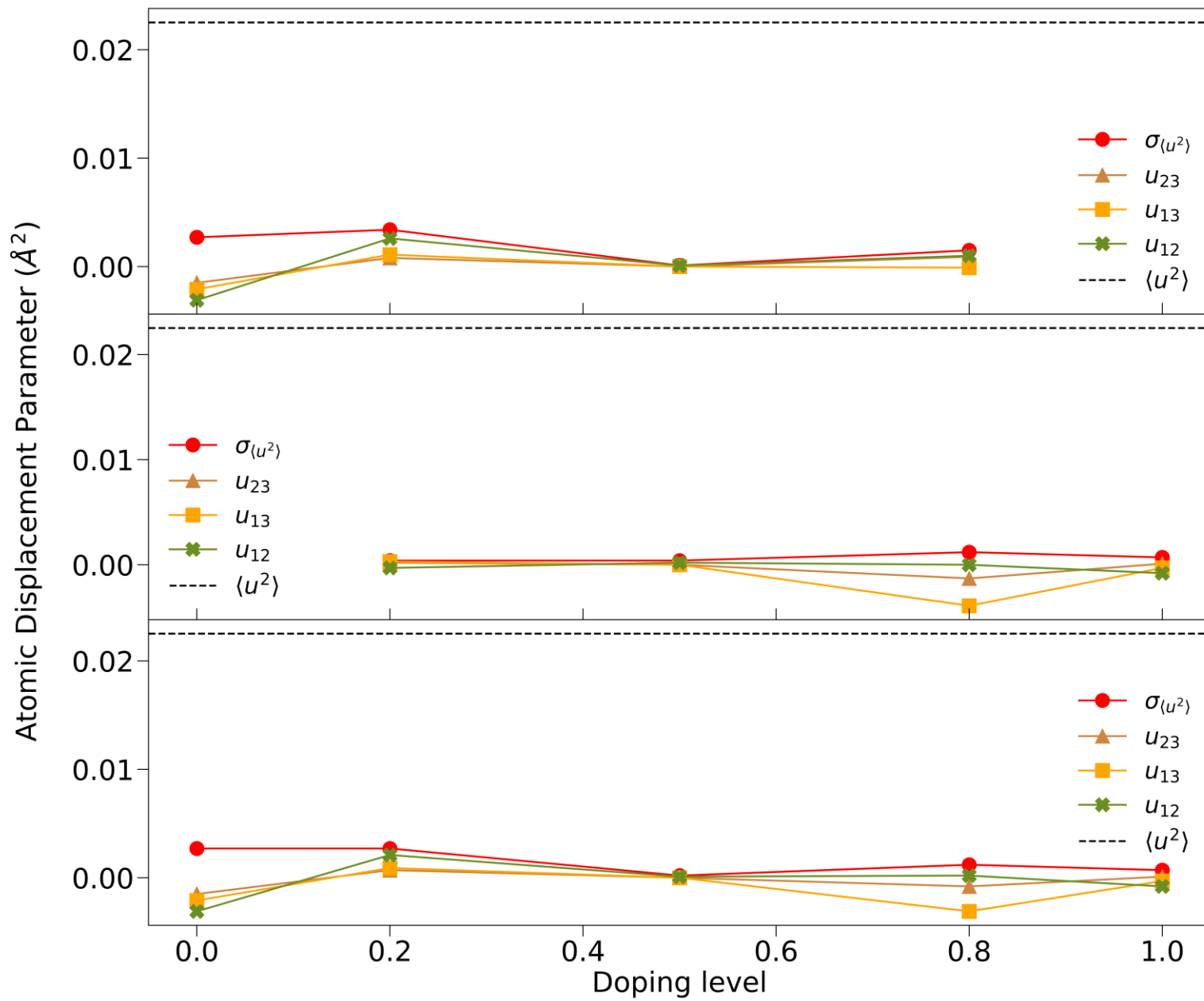






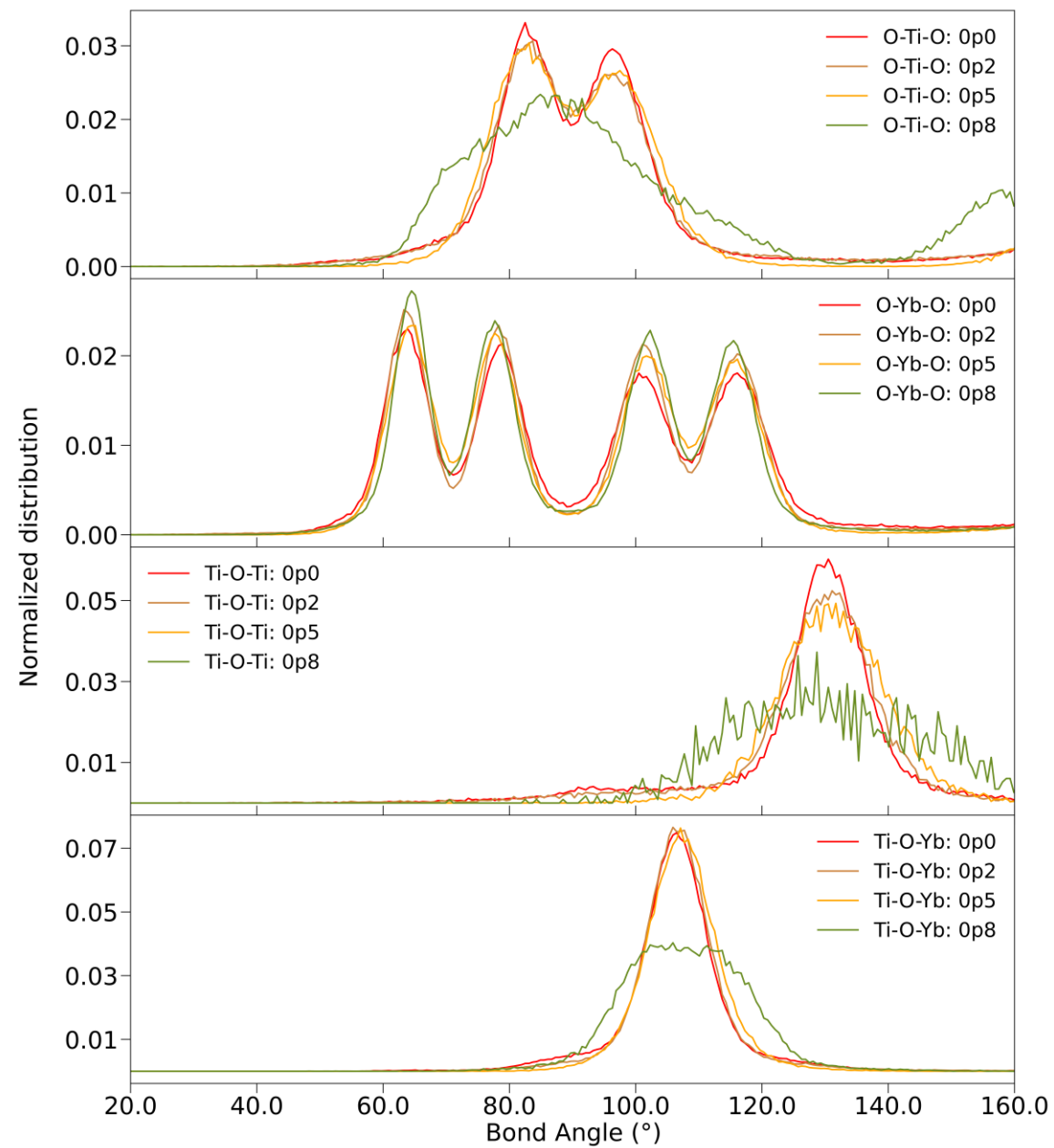


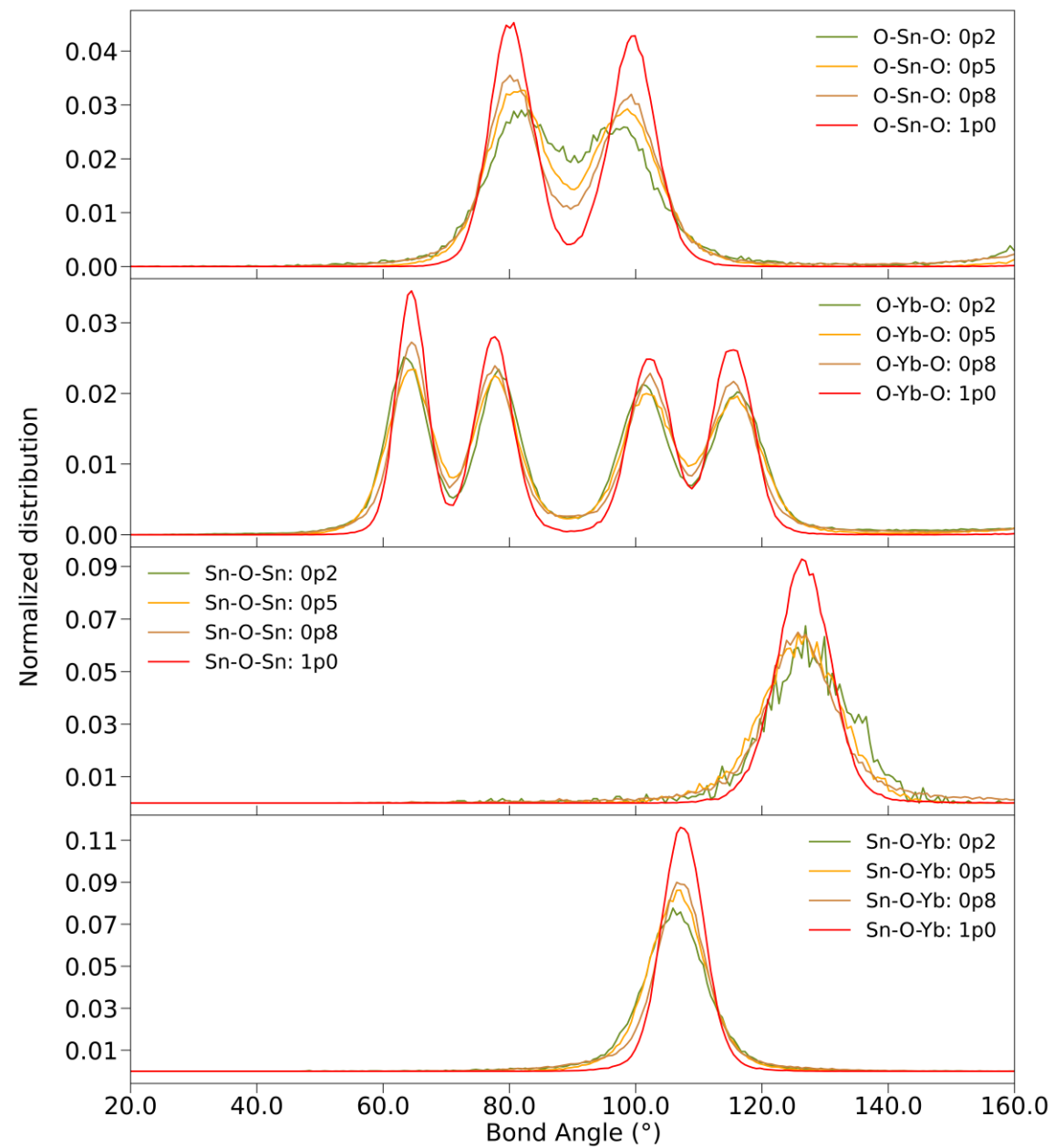
ADPs



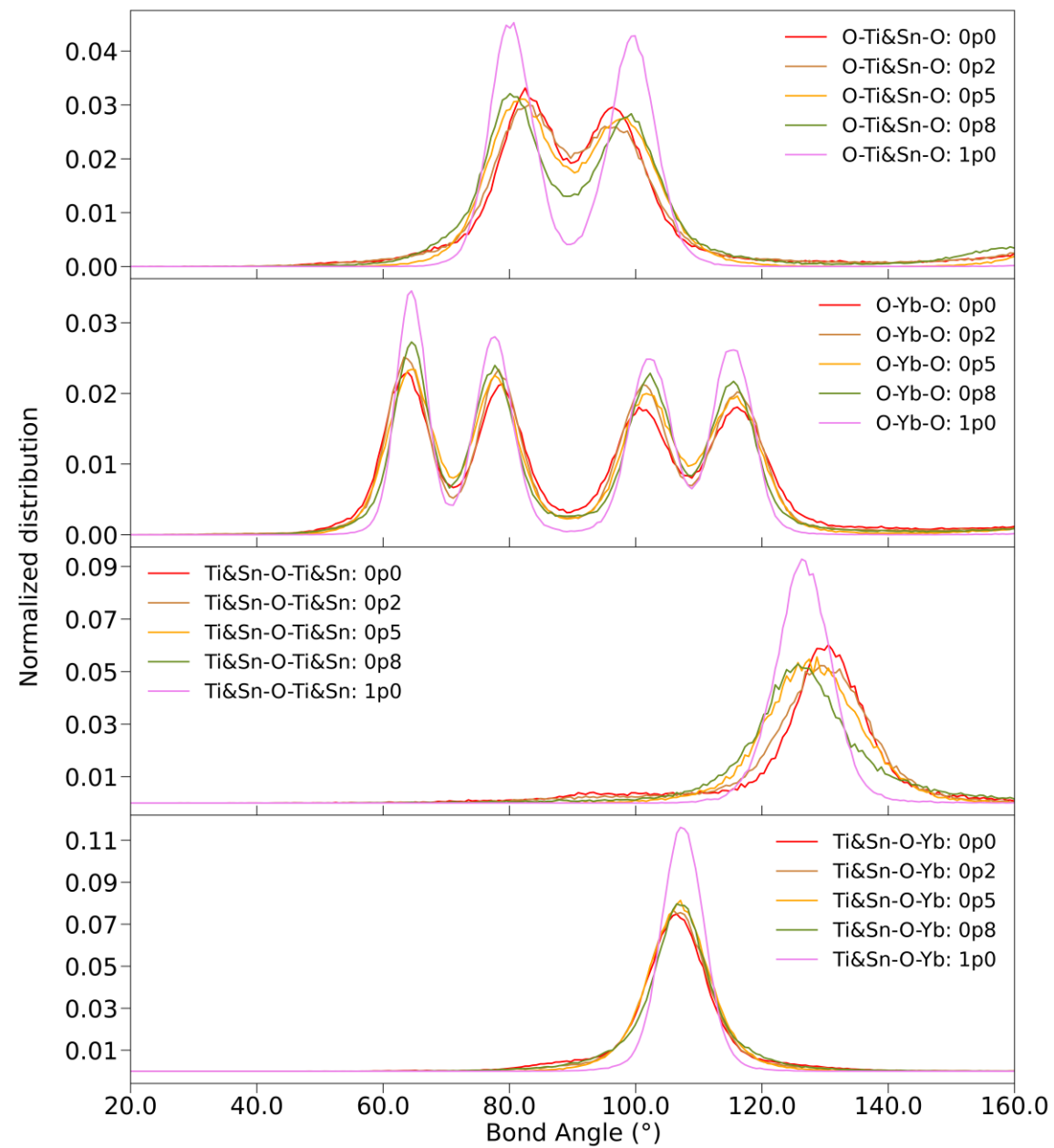
No obvious anisotropy was observed in all samples

Triplets bond angle distribution





Ti & Sn



- ❖ As the doping level increases, the distortion of the local TiO₆ octahedrons increases.
- ❖ Meanwhile, the relative orientation in between those corner sharing TiO₆ octahedrons is distorted as well.
- ❖ The Yb pyrochlore sublattice is well kept.
- ❖ Distortion of the local tetrahedral environment formed by Ti(Sn) and Yb is enhanced.
- ❖ The Sn-only involved angles *do not* show that obvious change as compared to those Ti-only involved angles.

- ❖ Consistence with other results?
- ❖ Multiple RMC runs to check self-consistenc