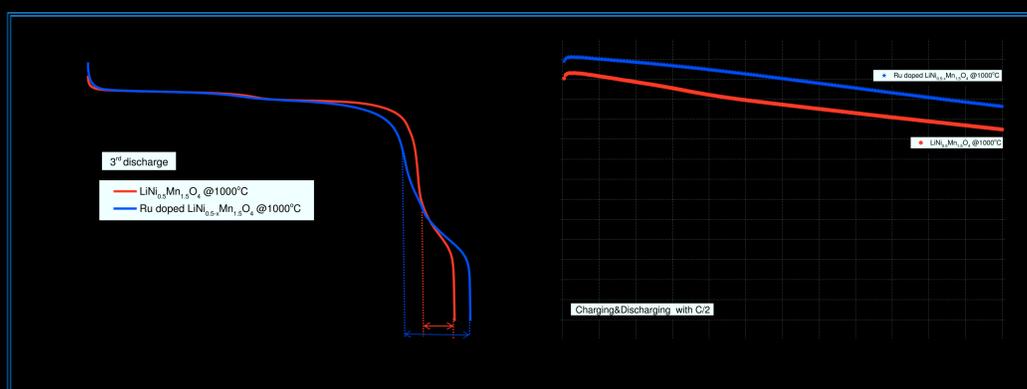


# Investigation of transition metal doping effect on $\text{LiNi}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$ spinel cathode by in-situ XRD studies during electrochemical cycling

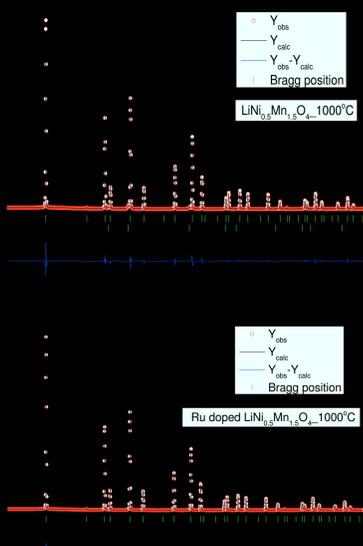
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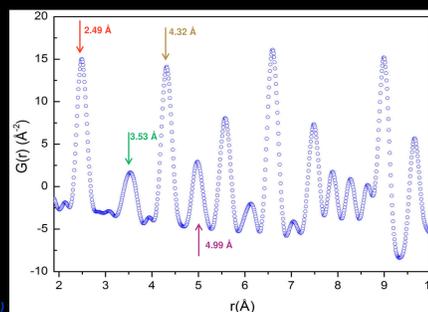
→ Even though Ru doped  $\text{LiNi}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$  @1000°C (blue curve) has larger 4V electrochemical activity than  $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$  @ 1000°C (red curve) which corresponds to the  $\text{Mn}^{3+}/\text{Mn}^{4+}$  electrochemical reaction, it has better capacity and cycling stability.



$a = 8.1789(1) \text{ \AA}$   
~5%  $\text{Li}_2\text{Ni}_2\text{O}_7$

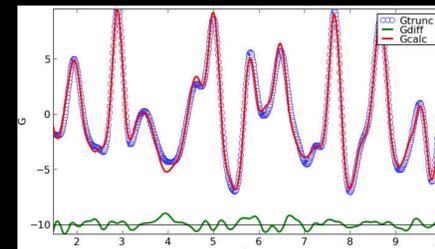
→ The impurity phase ( $\text{Li}_2\text{Ni}_2\text{O}_7$ ) vanishes after Ru-doping on  $\text{LiNi}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$

$a = 8.18885(4) \text{ \AA}$



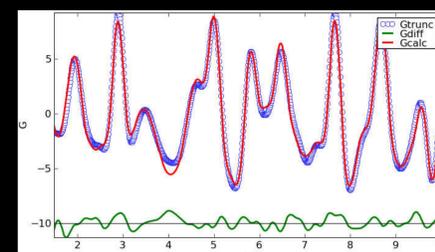
Pair Distribution Function (PDF) gives the probability of finding any two atoms separated by a distance  $r$ .

→ PDF peak position gives bond lengths directly  
→ Intensities of PDF peaks yield coordination numbers  
→ The PDF peak width gives information about atomic vibrations and disorder



$\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$  main phase : %91.5  
 $\text{Li}_2\text{Ni}_2\text{O}_7$  impurity : %8.5  
Rwp: %8.9

	$\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$		Ru-doped $\text{LiNi}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$	
	PDF	Rietveld	PDF	Rietveld
a (Å)	8.172	8.179	8.196	8.189
Metal-O (Å)	1.943	1.943	1.961	1.945



Ru-doped  $\text{LiNi}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$  main phase  
Rwp: %10.9

