Electronic Supplementary Material (ESI) for Environmental Science: Advances.

Supplementary Information (SI)

Synthesis and characterization of novel dual-capped Zn-urea nanofertilizers and application in nutrient delivery in wheat.

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Table SI 1: Main peaks identified by FTIR spectroscopy of dual-capped Zn NPs.

Functional Group/ Vibration	**Characteristic Absorption (cm^{-1})**	**NAC-SAL Zn-NP (cm^{-1})**	**NAC-Urea Zn-NP (cm^{-1})**	**SAL-Urea Zn-NP (cm^{-1})**
Aromatic C-H Bending	680-860	702, 746, 811	-	704, 758, 811
NO_3^-	800-860	834	835	835
Phenyl C-O	1100-1350	1127	-	1140
C-O-C asymmetric Stretch	1250	1255	-	1244
O-H	1260-1410	1355	1354	1354
C=C Stretch	1440-1625	1486, 1449	-	1487, 1457
Aromatic C=C Bending	1500 - 1700	-	-	1561
N-H Bending*	1550-1640	1596	1594	1603
C=O for Zn-carboxylic*	1600	1596	1594	1603
Amide C=O Stretch	1630 - 1690	-	1651	1660
Carboxylic Acid C=O Stretch	1710 - 1780	1790	1790	1790
Amine N-H Stretch	3300 - 3500	-	-	3358, 3463

*may be overlapping

Table SI 2: Fast Fourier Transform (FFT) convolution of dual capped Zn-based nanoparticles.

Product	(h k l)	Angle	Wulfingite $Zn(OH)_2$
	(2 1 1)	2.86 Å	2.72 Å
NAC-SAL Zn NP	(3 1 1)	2.20 Å	2.21 Å
	(2 2 1)	2.02 Å	2.01 Å
	(1 3 1)	1.59 Å	1.59 Å
	(2 1 1)	2.73 Å	2.72 Å
	(0 2 1)	2.29 Å	2.28 Å
SAL-Urea Zn NP	(2 2 1)	2.02 Å	2.01 Å
	(4 0 2)	1.6 Å	1.6 Å
	(5 2 0)	1.41 Å	1.41 Å
	(2 1 1)	2.92 Å	2.72 Å
	(0 2 0)	2.58 Å	2.58 Å
NAC-Urea Zn NP	(4 1 1)	1.83 Å	1.82 Å
	(1 3 0)	1.68 Å	1.68 Å
	(4 1 1)	1.56 Å	1.55 Å

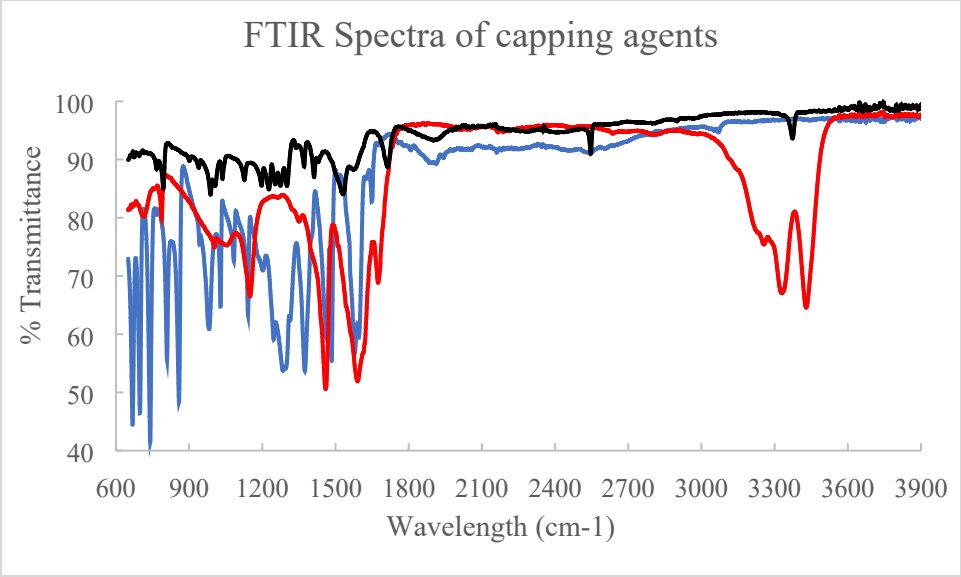

Figure SI 1: Infrared spectra of capping agents: (blue) sodium salicylate (SAL), (red) urea, and (black) n-acetyl cysteine (NAC).

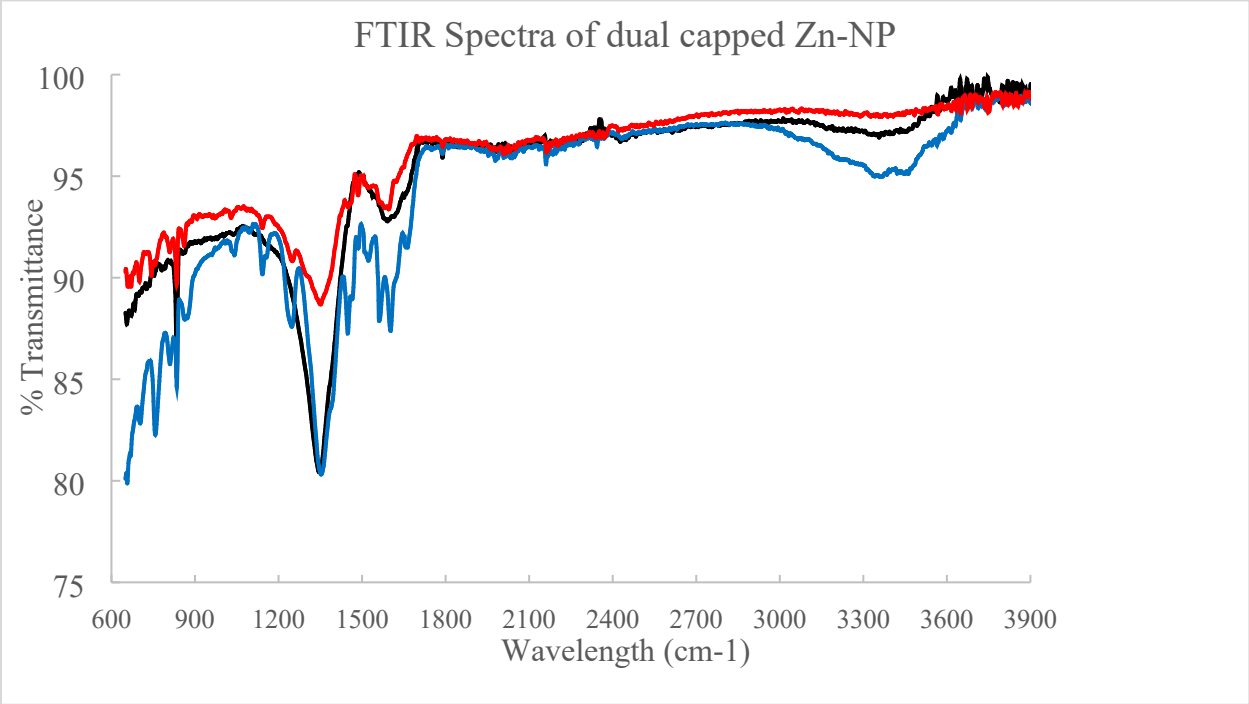

Figure SI 2: FTIR spectra of dual capped Zn nanoparticles: (black) NAC-Urea Zn NP, (blue) SAL-Urea Zn NP, and (red) NAC-SAL Zn NP.

Based on the crystal lattices distances (d-spacing) from HR-TEM, it was possible to match the crystalline structure of the samples with Wulfingite zinc hydroxide