

1 **Phytoremediation of soil contaminated with**
2 **lithium ion battery active materials – A proof of concept**
3 **study**

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16 Data provided in this supporting information describes detailed instrumental parameters for
17 inductively coupled plasma-optical emission spectroscopy (ICP-OES) and laser ablation-
18 inductively coupled plasma-mass spectrometry (LA-ICP-MS, see Tables S1 and S2).
19 Applied chemicals and materials are described in section S1.2. Section 2 shows photos,
20 microscopic, LA-ICP-MS and μ XRF images of *alyssum murale* at different stages of the
21 study (Figures S1-S5).

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23 **S1 Experimental**

24 **S1.1 Detailed instrumental parameters**

25 Table S1: ICP-OES measurement conditions for sample introduction and measured elements. The
26 emission lines used for the quantification of the respective element are highlighted in *italic*. Limit of
27 detection (LOD) and limit of quantification (LOQ) for ICP-OES are shown.

RF power / W	1400
Total argon flow rate / L min ⁻¹	13.65
Sample carrier gas flow rate / L min ⁻¹	0.85
Auxiliary plasma gas flow rate / L min ⁻¹	0.80
Plasma gas flow rate / L min ⁻¹	12.0
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Wavelength Li / nm	<i>670.780</i>
Ni / nm	<i>221.648, 231.604, 232.003</i>
Co / nm	<i>228.616, 230.786, 238.892</i>
Mn / nm	<i>257.611, 259.373, 260.569</i>
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LOD, LOQ Li / μ g L ⁻¹	0.3, 1.0
Ni / μ g L ⁻¹	0.2, 0.7
Co / μ g L ⁻¹	0.4, 1.3
Mn / μ g L ⁻¹	0.1, 0.3

28 **LOD, limit of detection; LOQ, limit of quantification**

29 Table S2: LA-ICP-MS parameters for elemental imaging of *alyssum murale* leaves.

LA (LSX-213, Teledyne CETAC)		ICP-MS (7700x-Series, Agilent)	
Spot size / μm	25	RF power / W	1550
Source pulse energy / %	100	Sampling depth / mm	6.0
Line spacing / μm	0	Total argon flow rate / L min^{-1}	15.00
Shot repetition rate / Hz	20	Additional carrier gas flow rate / L min^{-1}	0.95
Scan rate / $\mu\text{m s}^{-1}$	25	Auxiliary plasma gas flow rate / L min^{-1}	0.90
Gas flow (He) / mL min^{-1}	900	Integration time per mass / ms	50

30 **LA, Laser ablation; ICP-MS, inductively coupled plasma-mass spectrometry; RF, radio frequency**

31 S1.2 Chemicals and materials

32 $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$ hexahydrate (98 %, Alfa Aesar, Thermo Fisher Scientific, Waltham, MA, USA),
 33 $\text{CoSO}_4 \cdot 7\text{H}_2\text{O}$ (99+ %, Acros Organics, Thermo Fisher Scientific), $\text{MnSO}_4 \cdot \text{H}_2\text{O}$ (99+ %, Acros Organics, Thermo Fisher Scientific) and distilled water were used for the
 34 contamination study with irrigation water. ICP-OES external calibration was performed with
 35 ICP standards ($\text{Ni}(\text{NO}_3)_2$, $\text{Co}(\text{NO}_3)_2$, $\text{Mn}(\text{NO}_3)_2$ and LiNO_3 in 2.3 % HNO_3 , respectively
 36 (1000 mg L^{-1} , Merck, Darmstadt, Germany). Dilution of samples and calibration standards
 37 were conducted with 2 % HNO_3 (65-69 %, Suprapur[®], Merck) and deionized water (18.2 $\text{M}\Omega$
 38 cm^{-1} , TOC 2 mg L^{-1} , Millipore, Merck). $\text{LiNi}_{0.33}\text{Co}_{0.33}\text{Mn}_{0.33}\text{O}_2$ particles (Custom Cells GmbH,
 39 Itzehoe, Germany) were used for the direct soil contamination. Glacial acetic acid (VWR
 40 International GmbH, Darmstadt, Germany) was used for acidification of aqueous solutions
 41 for pH dependent dissolution experiments and helium (6.0, Westfalen AG, Münster,
 42 Germany) was applied for LA-ICP-MS measurements.
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44 S2 Hyperaccumulation of Ni, Co and Mn in *alyssum murale*



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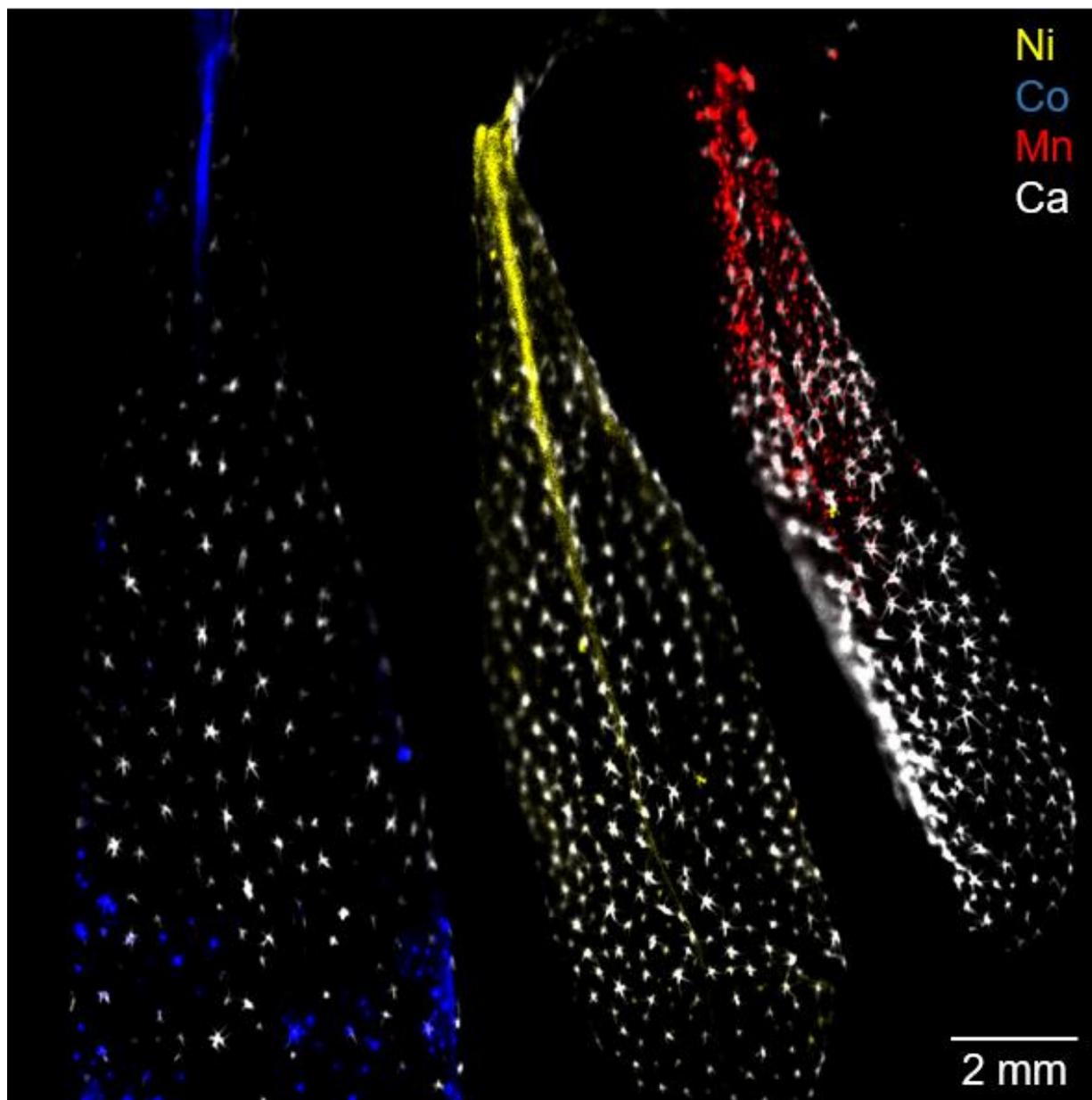
46 **Figure 1.** Reduced plant growth of *alyssum murale* with increased Ni concentration (from left to right:
 47 level 10, 50 and 250) at end the of the accumulation phase (day 46). Crystallization effects of $\text{Ni}(\text{NO}_3)_2$

48 from the irrigation water at the soil surface and the dieback of plants were observed for level 250
49 (right).



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51 **Figure 2.** Microscopic image of the leaf surface showing red dyed trichomes which indicates an
52 exocellular deposition of Co-rich minerals.



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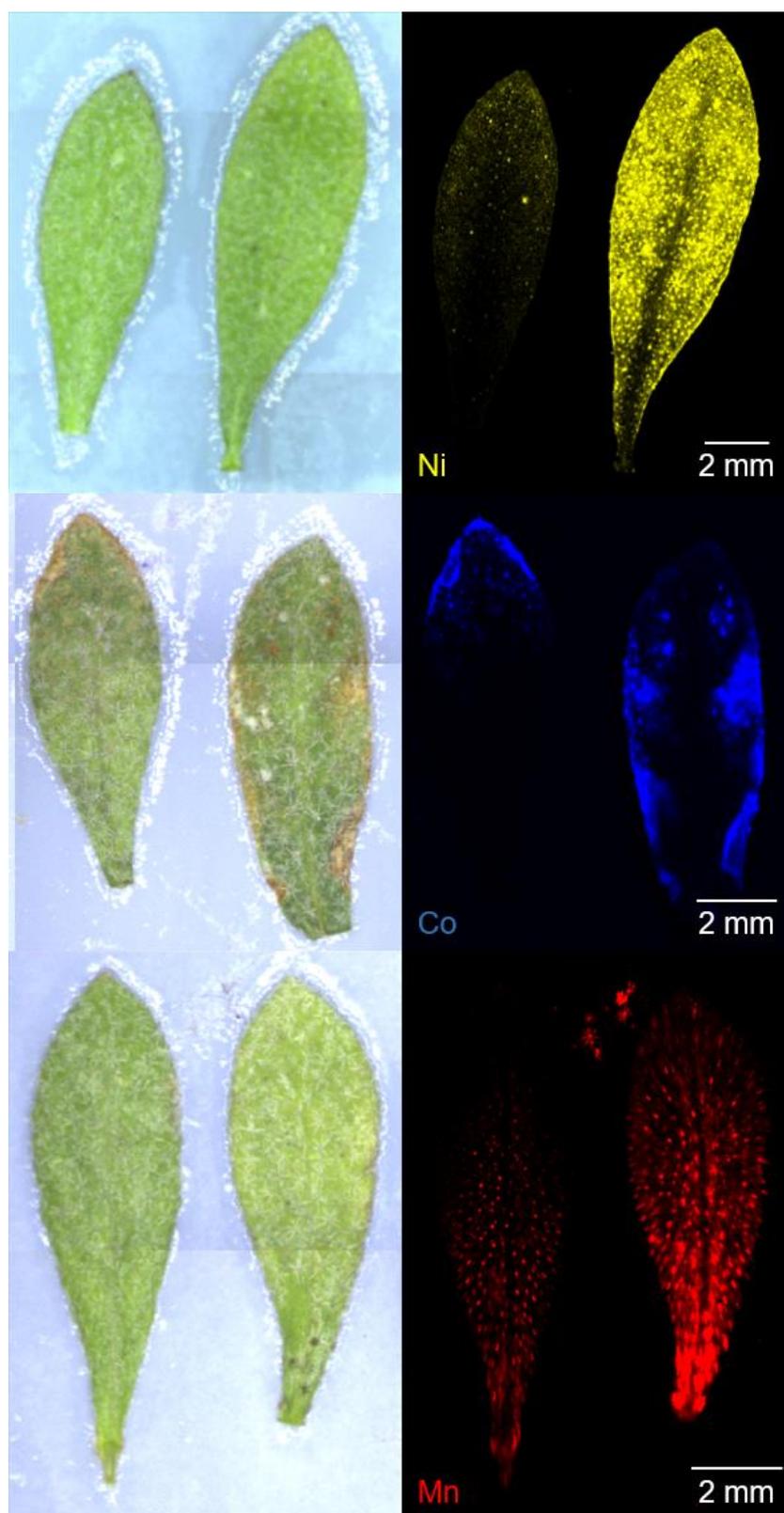
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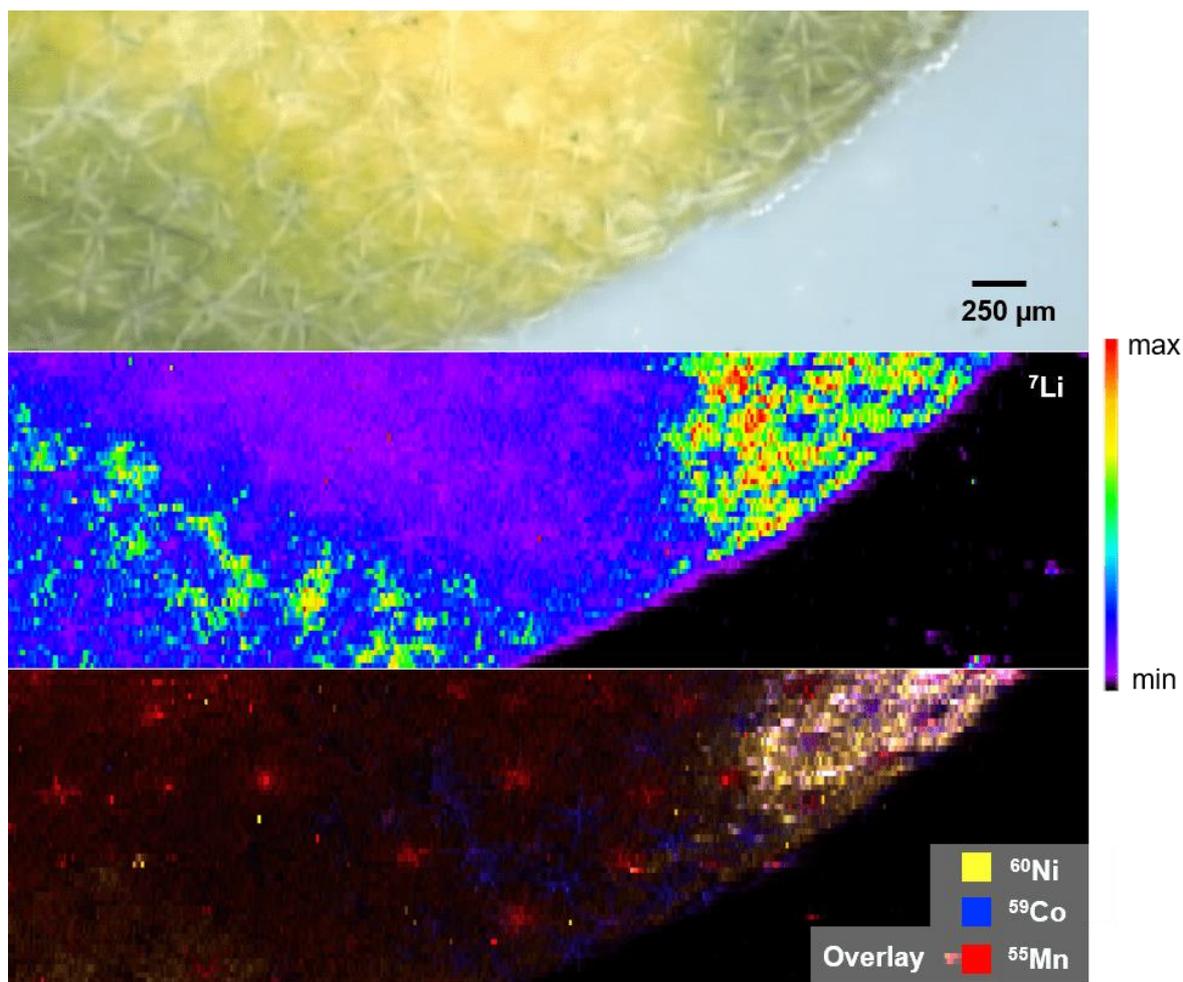
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Figure S3: μXRF overlay of the Ca signal (white) with the respective transition metals (Ni=yellow, Co=blue and Mn=red). Ca signals depict the trichome structures on the surface of the leaf and the occasional co-localization of Co with trichomes. Samples were measured five times and averaged. A spot size of 29 μm, a spot distance of 20 μm and a dwell time of 10 ms were used.



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Figure S4: Microscopic (left) and μ XRF (right) image of two *alyssum murale* leaves after 46 days of Ni (yellow), Co (blue) and Mn (red) contamination and accumulation. The left leaf was collected from a plant at the lowest contamination (level 1), the right leaf from contamination level 2. Samples were measured in three repetitions with a spot size of 29 μ m, a spot distance of 20 μ m and a dwell time of 26 ms.



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Figure 5. LA-ICP-MS image showing Li and transition metal distribution in an *alyssum murale* leaf with parched areas after contamination with LIB electrode material. Reduced Li signals in parched areas indicate a dissolved state in the cytosol.