# Contents

1 Motivation 1

2 Fundamentals of XAS 4
   2.1 The X-ray absorption process 4
   2.2 The XANES spectrum 5
      2.2.1 Qualitative interpretation of a XANES spectrum 7
      2.2.2 Quantitative interpretation of a XANES spectrum 8
   2.3 The EXAFS spectrum 10
      2.3.1 Quantitative interpretation of an EXAFS spectrum 12

3 Fundamentals of High Resolution X-ray Emission Spectroscopy (HRXES) 17
   3.1 Non-resonant HRXES 17
   3.2 Resonant HRXES 18
      3.2.1 Extended resonant HRXES 20

4 The experiments 25
   4.1 ANKA and DORIS III 25
   4.2 The INE-Beamline 25
      4.2.1 The measuring modes and the experimental set-up 27
      4.2.2 The Double Crystal Monochromator (DCM) 30
      4.2.3 The samples 32
   4.3 The W1 beamline 33

5 Lithium niobate 35
   5.1 Growth, defects and structure of the lithium niobate crystals 35
   5.2 Absorption spectra of lithium niobate from IR to hard X-ray regions 36
6 Doped lithium niobate

6.1 Copper-doped lithium niobate
   6.1.1 Introduction
   6.1.2 Preparation of the samples
   6.1.3 Experiment, methods and data evaluation
   6.1.4 Results and discussion
   6.1.5 Conclusion

6.2 Manganese-doped lithium niobate
   6.2.1 Introduction
   6.2.2 Samples
   6.2.3 Experimental details
   6.2.4 Results
   6.2.5 Discussion
   6.2.6 Conclusion

6.3 Iron-doped lithium niobate
   6.3.1 Introduction
   6.3.2 Samples
   6.3.3 Experimental details
   6.3.4 Results and discussions
   6.3.5 Conclusion

6.4 Bond Valence Model (BVM)

7 Lithium niobate irradiated with $^3\text{He}^{2+}$ ions

7.1 Introduction
7.2 Preparation of the samples
7.3 Experiment, methods and data evaluation
7.4 Results and discussion
   7.4.1 XANES analysis
   7.4.2 EXAFS analysis
7.5 Conclusion

8 Summary and outlook

A The studied LN cluster and graphical comparison of the Cu, Mn and Fe EXAFS results
B MoO$_3$ nanoparticles supported on Mesoporous SBA-15: Characterization of starting materials and the products using X-ray scattering, Physisorption, Transmission Electron microscopy, Raman and XAFS spectroscopy

B.1 Introduction ................................................................. 95
B.2 Experimental section ....................................................... 96
  B.2.1 Synthesis of pristine Mesoporous SBA-15 ....................... 96
  B.2.2 Synthesis of MoO$_3$/SBA-15 .................................. 96
B.3 Results and discussion ................................................... 98
  B.3.1 Powder X-ray Diffraction .................................... 98
  B.3.2 Raman spectroscopy ............................................. 100
  B.3.3 Nitrogen physisorption ....................................... 102
  B.3.4 Transmission Electron Microscopy and Scanning Electron Microscopy ... 103
  B.3.5 XAFS .......................................................... 103
B.4 Conclusion ............................................................. 111