
Table of contents

1	INTRODUCTION	1
2	FUNDAMENTALS	4
2.1	TRANSITION METAL DICHALCOGENIDES.....	4
2.1.1	<i>Crystal structure</i>	4
2.1.2	<i>Electronic structure</i>	7
2.1.3	<i>Synthesis.....</i>	9
2.2	THE INTERCALATION REACTION	10
2.2.1	<i>Definition and effects.....</i>	10
2.2.2	<i>Intercalation in alkali-containing solutions</i>	15
2.2.3	<i>Intercalation in UHV.....</i>	15
2.2.4	<i>Electrochemical intercalation and batteries</i>	16
2.3	MOTIVATION AND OUTLINE OF THE PRESENT WORK.....	22
3	EXPERIMENTAL.....	24
3.1	PHOTOELECTRON SPECTROSCOPY	24
3.1.1	<i>Basics</i>	25
3.1.2	<i>The photon sources.....</i>	27
3.1.3	<i>The electron analyzer</i>	28
3.1.4	<i>Spectra and interpretation.....</i>	29
3.2	UHV EQUIPMENT AND SPECTROMETER SYSTEMS	35
3.2.1	<i>The ESCALab Mk II.....</i>	36
3.2.2	<i>The integrated system</i>	36
3.2.3	<i>BESSY.....</i>	37
3.2.4	<i>Preparation chambers</i>	38
3.3	PREPARATIVE METHODS	40
3.3.1	<i>Samples</i>	40
3.3.2	<i>Sources</i>	40
3.4	EX-SITU CHARACTERIZATION TECHNIQUES.....	42
3.4.1	<i>AFM</i>	42
3.4.2	<i>TEM</i>	42
4	THIN FILM SYNTHESIS.....	44
4.1	LOW-PRESSURE GROWTH TECHNIQUES	44
4.2	THE ELECTRONIC STRUCTURE OF TiX_2	45
4.3	OPTIMIZATION.....	47
4.3.1	<i>Precursors.....</i>	47
4.3.2	<i>Substrate.....</i>	48
4.3.3	<i>Pressure and temperature</i>	53
4.4	THE REACTION MECHANISM.....	58
4.5	EX-SITU CHARACTERIZATIONS	61
5	INTERCALATION.....	66
5.1	DEPOSITION ON SINGLE CRYSTALS	66
5.1.1	<i>Na/TiS₂</i>	66
5.1.2	<i>Na/TiSe₂</i>	78
5.1.3	<i>Na/1T-TaS₂.....</i>	86
5.1.4	<i>Na/1T-TaSe₂.....</i>	90
5.2	CO-DEPOSITION EXPERIMENTS.....	92
5.2.1	<i>Na, Li and Cs/1T-TaSe₂.....</i>	93
5.2.2	<i>Halogens and Na</i>	99
5.2.3	<i>Discussion: electrostatic fields and relative intercalation strengths.....</i>	100
5.3	DEPOSITION ON THIN FILMS	102
5.4	IN-SITU ELECTROCHEMICAL INTERCALATION	109

5.4.1	<i>The electrolyte</i>	109
5.4.2	<i>Sample preparation</i>	109
5.4.3	<i>Results</i>	113
6	DISCUSSION AND CONCLUSIONS	123
6.1	BINDING ENERGY SHIFTS AND CHARGE TRANSFER.....	123
6.2	THE IONIC AND ELECTRONIC CONTRIBUTIONS TO THE ELECTROCHEMICAL POTENTIAL	126
6.3	SUMMARY OF RESULTS AND PERSPECTIVES	129
	REFERENCES	132
	LIST OF ABBREVIATIONS	141