

Contents

1	Introduction	1
2	Experimental Methods	11
2.1	Scanning Tunneling Microscopy (STM)	11
2.2	Scanning Tunneling Spectroscopy (STS)	16
2.3	Spin-Polarized STM	17
2.3.1	Single Atom Magnetization Curves (SAMCs) Extracted from dI/dV Maps	21
2.4	Inelastic Scanning Tunneling Spectroscopy (ISTS)	22
2.5	Experimental Setup	26
2.6	Design and Construction of an XSTM head	27
3	Model Descriptions of Single and Coupled Magnetic Atoms	31
3.1	Model Calculations for Quantum Spins: Excitations and Mag- netization	31
3.1.1	Introduction of the model for ISTS	32
3.1.2	Connection to Other Models	38
3.1.3	ISTS with Spin-Polarized Tips	39
3.1.4	The Inelastic Contribution to ISTS at Low Temperature	40
3.1.5	100 % Spin-Polarized Sources of Tunneling Electrons . .	43
3.1.6	Excitations of Coupled Spin Systems	45
3.1.7	Numerical Implementation	48
3.2	Comparison of Quasi-Classical Heisenberg Model and Ising Model	50
3.2.1	Numerical Implementation	55
4	Isolated Spins on Semiconductor Surfaces	59
4.1	Introduction: Magnetic Atoms on (110) Surfaces of III-V Semi- conductors	60
4.2	Experiments: Fe on InSb(110)	63
4.2.1	Preparation and Characterization of the Sample System	63
4.2.2	Density Functional Calculations	67

4.2.3	ISTS	69
4.2.4	The Landau Level Asymmetry	74
4.2.5	Landau Level Asymmetry with Spin-Polarized Tips . . .	77
4.3	Discussion	81
4.3.1	The Hypothesis $S = 1$	83
4.3.2	The Hypothesis $S \neq 1$	95
4.4	Conclusions and Outlook	99
5	Single Magnetic Atoms on Metallic Substrates	103
5.1	Introduction: Magnetic Atoms on Noble Metal (111) Surfaces .	104
5.2	Tip and Sample Preparation	105
5.3	SAMCs of Fe on Cu(111)	106
5.4	Simulated Distributions of the Fitted Effective Magnetic Moment	108
5.5	ISTS on Single Fe Atoms on Cu(111)	110
5.6	ISTS on Single Fe Atoms on Ag(111)	113
5.7	Tight Binding and Ab Initio Calculations of Magnetization Ex-	
	citations	116
5.8	Discussion	118
5.9	Comparison of Single Atom Magnetism on Different Substrates .	119
6	Magnetic Nanostructures Constructed from Individual Atoms	123
6.1	Lateral Manipulation	124
6.2	Introduction: SAMCs of RKKY-Coupled Magnetic Nanostruc-	
	tures	127
6.3	Pair Magnetization Curves	130
6.4	Chains of AFM Coupled Fe Atoms	135
6.5	The Magnetic ‘Flower’ Structure	142
6.6	Atomic Scale Spin Logic Devices	146
6.6.1	Illustration of the Concept	146
6.6.2	Experimental Realization	148
6.6.3	SAMCs of the Spin Leads	152
6.6.4	Comparison to Ising Model Calculations	154
6.7	Summary and Outlook	158
A	Lemmata and Proofs	159
A.1	Proof of Theorem 1	159
A.2	Proof of Theorem 2	163
A.3	Lemmata	165
A.3.1	Symmetry Properties of \hat{H} at $\mathbf{B} = 0$	165

A.3.2 Lemma 3	166
A.3.3 Lemma 4	166
A.3.4 Lemma 5	169
A.3.5 Lemma 6	170
A.3.6 Lemma 7	171
Bibliography	175
Publications	188
Acknowledgements	190