

Contents

Introduction	II
1 Density functional theory (DFT)	7
1.1 Overview	7
1.2 Origin of DFT	8
1.3 The Kohn-Sham equations	10
1.4 Spin Density Functional Theory	11
1.5 Approximations made to the exchange-correlation term E_{XC}	12
2 The FLAPW method	15
2.1 The generalized eigenvalue problem	15
2.2 From augmented planewaves (APW) to Linearized (L)APW	17
2.3 The Full-Potential LAPW	19
2.3.1 Film Calculations within FLAPW	22
2.4 The Kohn-Sham-Dirac Equation	24
2.4.1 The Scalar Relativistic Approximation	25
3 Magnetism of low dimensional systems	29
3.1 Stoner Model	30
3.1.1 Role of coordination number:	33
3.2 Heisenberg Model and Beyond	34
3.3 Non-Collinear Magnetism	36
3.3.1 The Spin Space Groups	37
3.3.2 Spin Spirals	38
3.3.3 Generalized Bloch Theorem	39
3.3.4 Non-Collinear Magnetism in FLAPW	41
3.4 Magnetic Anisotropy	43
3.4.1 Magnetic anisotropy and critical temperature:	49
4 Collinear magnetism of 3d-monolayers on Rh substrates	51
4.1 3d-Monolayers on (001) oriented substrates	51
4.1.1 3d monolayers on Pd, Ag and W (001) substrates:	51
4.2 Results of 3d-Monolayers on Rh(001) Substrate	54

4.2.1	Relaxations and magnetic moments:	55
4.2.2	Magnetic order:	57
4.2.3	Magnetocrystalline anisotropy:	61
4.3	3 <i>d</i> -Monolayers on Rh(111) Substrate:	66
4.3.1	Relaxations and magnetic moments:	66
4.3.2	Magnetic order:	69
5	Fe monolayers on hexagonal nonmagnetic substrates	73
5.1	Results of Fe monolayer on different hexagonal substrates from collinear calculations:	74
5.1.1	Structural optimization & relaxations:	75
5.1.2	Magnetic order:	77
5.2	Results of Fe monolayer on different hexagonal substrates from non-collinear calculations:	79
5.2.1	Model Hamiltonian & Heisenberg model for 2D hexagonal lattices:	79
5.2.2	Results of Fe monolayer on Rh(111):	86
5.2.3	Results for the Fe monolayer on Tc(0001) substrate:	93
5.2.4	Comparison of Fe magnetic order on 4 <i>d</i> hexagonal substrates:	95
6	Co MCA from monolayers to atomic chains	103
6.1	Relaxations and magnetic order:	103
6.2	MCA of Co monolayer on 4 <i>d</i> substrates:	105
6.3	Co atomic chain on Rh(664):	108
6.3.1	Theoretical model and relaxation results:	108
6.3.2	Magnetocrystalline anisotropy:	110
	Summary and Conclusions	114
	Appendix	118
	Bibliography	127
	Acknowledgement	141