Contents

Chapter 1	introduction		
	1	Clusters and Nanoparticles	Ī
	2	Feynman's Vision	2
Chapter 2	Bulk and Interface		4
	1	Gradients Near Surfaces	4
	2	The Coordination Number Rules the Game	(
	3	Surface Science, a Source of Information for	
		Nanoscience	8
	4	Particle Size and Microstrain	11
	5	Biomimetics: Nature as a Source of Inspiration for	
		Strategies in Nanotechnology	17
Chapter 3	Geometric Structure, Magic Numbers, and Coordination		
_		umbers of Small Clusters	21
	1	The Consequences of the Range of the Radial Potential	
		Energy Function	21
	2	Magic Numbers by Geometric Shells Closing	26
	3	Magic Numbers by Electronic Shells Closing	29
	4	Cohesive Energy and Coordination Number	34
Chapter 4	E	ectronic Structure	41
•	1	Discrete States Versus Band Structure	41
	2	The Effects of Dimensionality and Symmetry in	
		Quantum Structures	42
	3	The Nonmetal-to-Metal Transition	47
		3.1 General Criteria	47
		3.2 The Special Case of Divalent Elements	49
		3.3 Experimental Criteria of Metallic Behaviour	51

x Contents

	4	Work Function, Ionisation Potential and Electron	55
	5	Affinity Electronic Structure of Semiconductor and Metal	33
	J	Clusters	60
		5.1 Optical Transitions in Semiconductor Nanoclusters	60
		5.2 Photochemical and Photophysical Processes of	00
		Semiconductor Nanoparticles	65
		5.3 Optical Properties of Metal Nanoclusters	69
	6	A Semiconductor Quantum Dot Electronic Device	74
		•	
Chapter 5		agnetic Properties	81
	Ì	A Brief Primer on Magnetism	81
		1.1 The Basic Parameters	81
		1.2 Curie Paramagnetism	82
		1.3 Curie–Weiss Paramagnetism	83
		1.4 Antiferromagnetism	84
		1.5 Ferromagnetism and Ferrimagnetism	84
		1.6 Molecular Magnets	86
		1.7 Superparamagnetism	88
		1.8 Other Forms of Magnetism	90
	2	The Concept of Frustration	91
	3	Magnetic Properties of Small Clusters	95
		3.1 Theoretical Predictions	95
		3.2 Experimental Observations of Magnetism in	
		Clusters	100
	4	Ferromagnetic Order in Thin Films and Monoatomic	
		Chains	106
	5	Finite Size Effects in Magnetic Resonance Detection	109
		5.1 Nuclear Magnetic Resonance	109
		5.2 Electron Spin Resonance	111
Chapter 6	TI	nermodynamics for Finite Size Systems	119
Chapter 0	1	Limitations of Macroscopic Thermodynamics	119
	1	1.1 A Formal Approach	119
		1.2 Systems Beyond the Thermodynamic Limit	120
			120
	2	1.3 The Breakdown of the Concept of Phases	124
	2	The Basics of Capillarity	124
		Phase Transitions of Free Liquid Droplets	120
	4	The Lotus Effect	136
	5	Classical Nucleation Theory	130
	6	Shape Control of Nanocrystals	
	7	Size Effects on Ion Conduction in Solids	148
	×	Principles of Self-Assembly	17/

Contents xi

Chapter 7	Adsorption, Phase Behaviour and Dynamics of Surface			
	Layers and in Pores	163		
	1 Surface Adsorption and Pore Condensation	163		
	1.1 The Langmuir Adsorption Isotherm	163		
	1.2 The Brunauer–Emmett–Teller (BET) Equation	163		
	1.3 Adsorption in Micropores	166		
	1.4 Adsorption and Condensation in Mesopores	168		
	1.5 Determination of Mesopore Volumes and Mean Pore Size	169		
	2 Adsorption Hysteresis and Pore Criticality	170		
	3 The Melting Point of Pore-confined Matter	178		
	4 Layering Transitions	185		
	4.1 Layering of Solids and Liquids Adsorbed on Smooth Surfaces	185		
	4.2 Layering Transitions of Confined Fluids in Smooth Pores	187		
	5 Liquid Coexistence and Ionic Solutions in Pores	191		
	6 The Effect of Pressure	193		
	7 Dynamics in Pores	194		
	7.1 Dielectric Properties	194		
	7.2 Diffusion and Viscosity Under Confinement	198		
Chapter 8	Nucleation, Phase Transitions and Dynamics of Clusters	209		
Chapter 6	1 Melting Point and Melting Enthalpy	209		
	1.1 Introduction	209		
	1.2 Supported Tin Clusters	210		
	1.2 Supported Till Clusters 1.3 Melting of Cadmium Sulfide Nanocrystals	210		
	1.4 Free Sodium Clusters	214		
	1.5 Isolated Silver Clusters	219		
		219		
	1.6 Simulated Melting Behaviour of Further Metal	221		
	Clusters	221		
	1.7 Discrete Periodic Melting of Indium Clusters	221		
	1.8 Hydrogen-Induced Melting of Palladium	222		
	Clusters	222		
	2 Dynamics of Metal Clusters	223		
Chapter 9	Phase Transitions of Two-Dimensional Systems	233		
<u></u>	1 Melting of Thin Layers	233		
	2 Structural Phase Transitions in Thin Layers	233		
	3 Glass Transition of a Polymer Thin Film	235		
	4 Surface Alloy Phases	236		
	T Surface (Moy 1 mases	250		

xii Contents

Chapter 10	Ca	italysis by Metallic Nanoparticles	239
	1	Some General Principles of Catalysis by Nanoparticles	239
	2	Size-Controlled Catalytic Clusters	241
	3	Shape-Dependent Catalytic Activity	246
	4	The Effect of Strain	248
	5	The Effect of Alloying	252
	6	Metal-Support Interaction	255
	7	The Influence of External Bias Voltage	257
Chapter 11	Aŗ	pplications: Facts and Fictions	263
	1	Nanomaterials	263
		1.1 General Considerations	263
		1.2 Applications in Medicine	263
		1.3 Intelligent Surfaces	265
		1.4 Applications in Catalysis	265
		1.5 Applications in Environmental Technologies	265
	2	Nanotechnology	266
		2.1 Applications to Nanomechanics	267
		2.2 Applications in Nanoelectronics	269
		2.3 Applications of Single Spin- and Nanomagnetism	272
		2.4 Applications of Optical Properties	273
	3	Hopes, Hazards and Hype	275
		3.1 Is Nanotechnology Useful?	275
		3.2 Potential Health and Environmental Hazards	276
		3.3 Ethical and Social Threats from Nanotechnology	276
		3.4 Is Nanotechnology but Hype?	278
Subject Inde	ex		281