Pr	reface EU amounts of an income and a contract to with an original Adjusted to the contract of	viii
1	Heterogeneous Catalysis and a Sustainable Future	1
2	The Potential Energy Diagram	6
	2.1 Adsorption, 7	
	2.2 Surface Reactions, 11	
	2.3 Diffusion, 13	
	2.4 Adsorbate–Adsorbate Interactions, 15	
	2.5 Structure Dependence, 17	
	2.6 Quantum and Thermal Corrections to the Ground-State	
	Potential Energy, 20	
3	Surface Equilibria	26
	3.1 Chemical Equilibria in Gases, Solids, and Solutions, 26	
	3.2 The Adsorption Entropy, 31	
	3.3 Adsorption Equilibria: Adsorption Isotherms, 34	
	3.4 Free Energy Diagrams for Surface Chemical Reactions, 40	
	Appendix 3.1 The Law of Mass Action and the Equilibrium	
	Constant, 42	
	Appendix 3.2 Counting the Number of Adsorbate Configurations, 44	
	Appendix 3.3 Configurational Entropy of Adsorbates, 44	

4	Rate Constants	47
	 4.1 The Timescale Problem in Simulating Rare Events, 48 4.2 Transition State Theory, 49 4.3 Recrossings and Variational Transition State Theory, 59 	
	4.4 Harmonic Transition State Theory, 61	
5	Kinetics	68
	 5.1 Microkinetic Modeling, 68 5.2 Microkinetics of Elementary Surface Processes, 69 5.3 The Microkinetics of Several Coupled Elementary Surface Processes, 74 5.4 Ammonia Synthesis, 79 	
6	Energy Trends in Catalysis	85
	 6.1 Energy Correlations for Physisorbed Systems, 85 6.2 Chemisorption Energy Scaling Relations, 87 6.3 Transition State Energy Scaling Relations in Heterogeneous Catalysis, 90 6.4 Universality of Transition State Scaling Relations, 93 	
7	Activity and Selectivity Maps	97
	 7.1 Dissociation Rate-Determined Model, 97 7.2 Variations in the Activity Maximum with Reaction Conditions, 101 7.3 Sabatier Analysis, 103 7.4 Examples of Activity Maps for Important Catalytic Reactions, 105 7.4.1 Ammonia Synthesis, 105 7.4.2 The Methanation Reaction, 107 7.5 Selectivity Maps, 112 	
8	The Electronic Factor in Heterogeneous Catalysis	114
	 8.1 The <i>d</i>-Band Model of Chemical Bonding at Transition Metal Surfaces, 114 8.2 Changing the <i>d</i>-Band Center: Ligand Effects, 125 8.3 Ensemble Effects in Adsorption, 130 8.4 Trends in Activation Energies, 131 8.5 Ligand Effects for Transition Metal Oxides, 134 	
9	Catalyst Structure: Nature of the Active Site	138
	 9.1 Structure of Real Catalysts, 138 9.2 Intrinsic Structure Dependence, 139 9.3 The Active Site in High Surface Area Catalysts, 143 9.4 Support and Structural Promoter Effects, 146 	

10	Poisoning and Promotion of Catalysts	150
11	Surface Electrocatalysis	155
	11.1 The Electrified Solid–Electrolyte Interface, 156	
	11.2 Electron Transfer Processes at Surfaces, 158	
	11.3 The Hydrogen Electrode, 161	
	11.4 Adsorption Equilibria at the Electrified Surface–Electrolyte Interface, 161	
	11.5 Activation Energies in Surface Electron Transfer Reactions, 162	
	11.6 The Potential Dependence of the Rate, 164	
	11.7 The Overpotential in Electrocatalytic Processes, 167	
	11.8 Trends in Electrocatalytic Activity: The Limiting Potential Map,	169
12	Relation of Activity to Surface Electronic Structure	175
	12.1 Electronic Structure of Solids, 175	
	12.2 The Band Structure of Solids, 179	
	12.3 The Newns-Anderson Model, 184	
	12.4 Bond-Energy Trends, 186	
	12.5 Binding Energies Using the Newns-Anderson Model, 193	
Ind	ex	195