

CONTENTS

CONTRIBUTORS	ix
INTRODUCTION THE WORLD OF OXIDE NANOMATERIALS <i>José A. Rodríguez and Marcos Fernández-García</i>	1
PART I BASIC CONCEPTS	7
Chapter 1. Theory of Size, Confinement, and Oxidation Effects <i>Chang Q. Sun</i>	9
Chapter 2. On Aqueous Interfacial Thermodynamics and the Design of Metal-Oxide Nanostructures <i>Lionel Vayssieres</i>	49
PART II SYNTHESIS AND PREPARATION OF NANOSTRUCTURED OXIDES	79
Chapter 3. Synthesis of Metal-Oxide Nanoparticles: Liquid–Solid Transformations <i>Lawrence D’Souza and Ryan Richards</i>	81
Chapter 4. Synthesis of Metal-Oxide Nanoparticles: Gas–Solid Transformations <i>S. Buzby, S. Franklin, and S. Ismat Shah</i>	119
PART III STUDY AND CHARACTERIZATION OF NANOSTRUCTURED OXIDES	135
Chapter 5. Techniques for the Study of the Structural Properties <i>José A. Rodríguez, Marcos Fernández-García, Arturo Martínez-Arias, and Jonathan C. Hanson</i>	137
Chapter 6. Techniques for the Study of the Electronic Properties <i>Marcos Fernández-García and José A. Rodríguez</i>	165

vi CONTENTS

Chapter 7. Post Hartree-Fock and Density Functional Theory Formalisms	185
<i>Francesc Illas and Gianfranco Pacchioni</i>	
Chapter 8. Parametric Quantum Methods in Modeling Metal Oxide Nanoclusters and Surfaces	217
<i>F. Ruelle and M. Sánchez</i>	
Chapter 9. Atomistic Models and Molecular Dynamics	247
<i>D.C. Sayle and T.X.T. Sayle</i>	
PART IV PHYSICOCHEMICAL PROPERTIES OF OXIDE NANOMATERIALS	287
Chapter 10. Theoretical Aspects of Oxide Particle Stability and Chemical Reactivity	289
<i>Ye Xu, William A. Shelton, and William F. Schneider</i>	
Chapter 11. Adsorption of Probe Molecules on Nanostructured Oxides	311
<i>James A. Anderson and Russell F. Howe</i>	
Chapter 12. Chemical Properties of Oxide Nanoparticles: Surface Adsorption Studies from Gas- and Liquid-Phase Environments	335
<i>John M. Pettibone, Jonas Baltrusaitis, and Vicki H. Grassian</i>	
Chapter 13. Transport Properties and Oxygen Handling	353
<i>Glenn C. Mather and Arturo Martínez-Arias</i>	
PART V INDUSTRIAL/TECHNOLOGICAL APPLICATIONS OF OXIDE NANOMATERIALS	379
Chapter 14. Adsorbents	381
<i>Pethaiyan Jeevanandam and Kenneth J. Klabunde</i>	
Chapter 15. Gas Sensors	411
<i>Doina Lutic, Mehri Sanati, and Anita Lloyd Spetz</i>	
Chapter 16. Photovoltaic, Photoelectronic, and Electrochemical Devices Based on Metal-Oxide Nanoparticles and Nanostructures	451
<i>Juan Bisquert</i>	
Chapter 17. Nanostructured Oxides in Photo-Catalysis	491
<i>Gerardo Colón-Ibáñez, Carolina Belver-Coldeira, and Marcos Fernández-García</i>	

Chapter 18. Oxide Nanomaterials for the Catalytic Combustion of Hydrocarbons	563
<i>Ilenia Rossetti and Lucio Forni</i>	
Chapter 19. Nanostructured Oxides in DeNO_x Technologies	603
<i>Marcos Fernández-García, Arturo Martínez-Arias, and Javier Pérez-Ramírez</i>	
Chapter 20. Chemistry of SO₂ and DeSO_x Processes on Oxide Nanoparticles	633
<i>José A. Rodríguez</i>	
Chapter 21. H₂ Production and Fuel Cells	651
<i>Xianqin Wang and José A. Rodríguez</i>	
Chapter 22. Oxide Nanomaterials in Ceramics	683
<i>Vicente Rives, Raquel Trujillano, and Miguel A. Vicente</i>	
Index	715

