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Nota di contenuto	Computational Modeling for Homogeneous and Enzymatic Catalysis; Contents; Preface; List of Contributors; 1 Computational Insights into the Structural Properties and Catalytic Functions of Selenoprotein Glutathione Peroxidase (GPx); 1.1 Introduction; 1.2 Catalytic Functions; 1.2.1 Peroxidase Activity; 1.2.2 Reductase Activity; 1.3 Computational Details; 1.3.1 Computational Methods; 1.3.2 Computational Models; 1.4 Results and Discussion; 1.4.1 Refinement of the Active Site; 1.4.2 Catalytic Functions: Peroxidase Activity; 1.4.3 Catalytic Functions: Effect of the Surrounding Protein on the Peroxidase Activity1.4.3.1 Hydrogen Peroxide Coordination; 1.4.3.2 Formation of Selenenic Acid [E-Se-OH]; 1.4.4 Catalytic Functions: Reductase Activity; 1.4.4.1 Peroxynitrite/Peroxynitrous Acid (ONOO /ONOOH) Coordination; 1.4.4.2 Oxidation Pathway; 1.4.4.3 Nitration

Pathways; 1.5 Summary; References; 2 A Comparison of Tetrapyrrole Cofactors in Nature and their Tuning by Axial Ligands; 2.1 Introduction; 2.2 Methodology; 2.3 Comparison of the Intrinsic Chemical Properties of the Tetrapyrroles; 2.3.1 Introduction; 2.3.2 Spin States; 2.3.3 Tetrapyrroles Prefer Their Native Ions; 2.3.4 Cavity Size and Flexibility of the Tetrapyrroles; 2.3.5 Cytochrome-like Electron Transfer; 2.3.6 Stability of a Metal-Carbon Bond; 2.3.7 Metallation Reaction; 2.4 Tuning of Tetrapyrrole Structure and Function by Axial Ligands; 2.4.1 Introduction; 2.4.2 Importance of the Lower Axial Ligand for B(12) Chemistry; 2.4.3 Lower Axial Ligand in Cofactor F430; 2.4.4 Importance of Axial Ligands for the Globins; 2.4.5 Role of Axial Ligands for the Cytochromes; 2.4.6 Role of the Axial Ligand in Heme Enzymes; 2.4.7 Tuning the His Ligand by Hydrogen Bonds in Heme Proteins; 2.4.8 Axial Ligand in Chlorophylls; 2.5 Concluding Remarks; References; 3 Modeling of Mechanisms for Metalloenzymes where Protons and Electrons Enter or Leave; 3.1 Introduction; 3.2 Energy Diagrams; 3.2.1 Photosystem II; 3.2.2 Cytochrome c Oxidase; 3.2.3 Nitric Oxide Reduction; 3.2.4 NiFe-hydrogenase; 3.2.5 Molybdenum CO Dehydrogenase; 3.3 Conclusions; References; 4 Principles of Dinitrogen Hydrogenation: Computational Insights; 4.1 Introduction; 4.2 Reaction Mechanism of the Coordinated Dinitrogen Molecule in Di-zirconocene-N(2) Complexes with a Hydrogen Molecule; 4.2.1 Mechanism of the Reaction (3); 4.2.2 Mechanisms of the Reactions (4) and (5); 4.3 Factors Controlling the N(2) Coordination Modes in the Di-zirconocene-N(2) Complexes; 4.4 Why the  $[(\eta^5\text{-C}_5\text{Me}_5)_2\text{Ti}(\text{N}_2)]$  Complex Cannot Add a H(2) Molecule to the Side-on Coordinated N(2), while its Zr- and Hf-analogs Can; 4.4.1 Relative Stability of the Lowest Singlet (S) and Triplet (T) Electronic States of the Complexes  $[(\eta^5\text{-C}_5\text{Me}_5)_2\text{M}(\text{N}_2)]$  (for M = Ti, Zr, and Hf, and n = 0 and 4)

## Sommario/riassunto

Here, the world's most active and productive computational scientists from academia and industry present established, effective and powerful tools for understanding catalysts. With its broad scope -- nitrogen fixation, polymerization, C-H bond activation, oxidations, biocatalysis and much more -- this book represents an extensive knowledge base for designing efficient catalysts, allowing readers to improve the performance of their own catalysts.