

1. Record Nr.	UNISA990000794750203316
Titolo	L'educazione dei figli
Pubbl/distr/stampa	Scandicci : La nuova Italia
Descrizione fisica	v. ; 24 cm
Collana	Biblioteca di scienze dell'educazione
Disciplina	649.109
Soggetti	Famiglie -- Educazione -- Storia
Collocazione	II.4. Coll.23/ 1/(VI B Coll. 77/24)L.M.
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia
2. Record Nr.	UNINA990004241910403321
Autore	Byron, George Gordon
Titolo	Alas! The love of women! : 1813-1814 / edited by Leslie A. Marchand
Pubbl/distr/stampa	London : Murray, 1974
ISBN	0-7195-2989-1
Descrizione fisica	XIV, 285 p. ; 23 cm
Locazione	FLFBC
Collocazione	P.3 BR.C.1332(3)
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia

3. Record Nr.	UNINA9910830195903321
Titolo	Computational modeling for homogeneous and enzymatic catalysis [[electronic resource] ] : a knowledge-base for designing efficient catalysts / / edited by Keiji Morokuma and Djamaladdin G. Musaev
Pubbl/distr/stampa	Weinheim, : Wiley-VCH Chichester, : John Wiley [distributore], 2008
ISBN	1-282-37223-8 9786612372230 3-527-62196-2 3-527-62197-0
Descrizione fisica	1 online resource (400 p.)
Altri autori (Persone)	MorokumaK <1934-> (Keiji) MusaevDjamaladdin G
Disciplina	660.2995
Soggetti	Catalysis - Computer simulation Catalysts
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
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  $[(\eta^5\text{-C}_5\text{Me}_n\text{H}_{5-n})_2\text{Ti}]$   
 $(\eta^2, \eta^2, \eta^2)\text{-N}_2$  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  $[(\eta^5\text{-C}_5\text{Me}_n\text{H}_{5-n})_2\text{M}]$   
 $(\eta^2, \eta^2, \eta^2)\text{-N}_2$ , II\_M (for M = Ti, Zr, and Hf, and n = 0 and 4)

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## 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.

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